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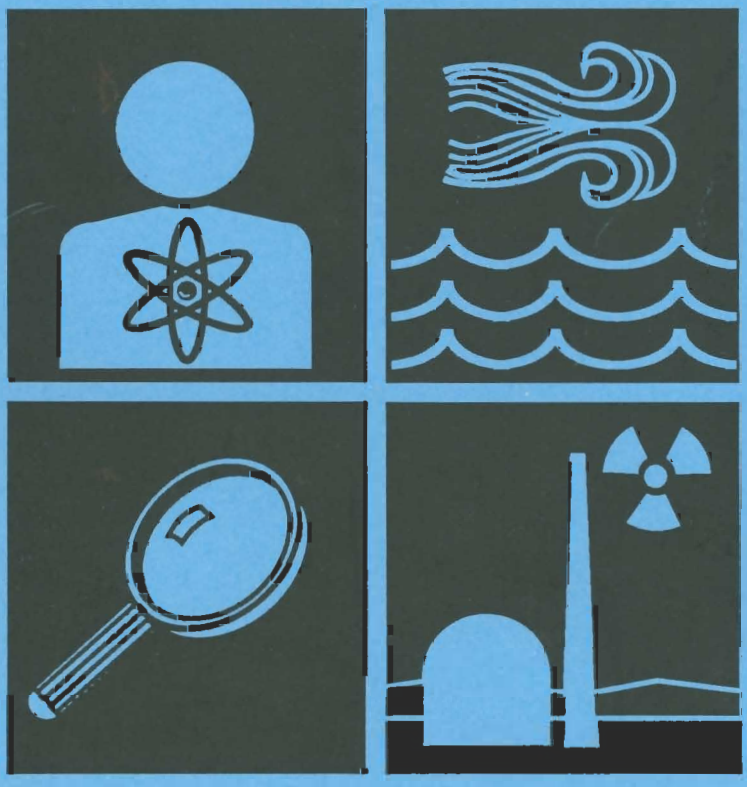
Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)

J. V. Ramsdell, Jr.
C. A. Simonen
K. W. Burk

February 1994



Prepared for the Technical Steering Panel
and the Centers for Disease Control and Prevention
under Contract 200-92-0503(CDC)/18620(BNW)

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PNWD-2224 HEDR

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Hanford Environmental Dose Reconstruction Project

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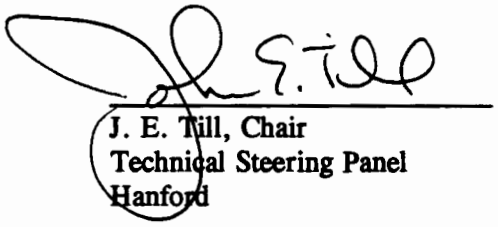
approved by the Technical Steering Panel.



J. E. Till, Chair
Technical Steering Panel
Hanford

January 17, 1994
Date

Preface

In 1987, the U.S. Department of Energy (DOE) directed the Pacific Northwest Laboratory, which is operated by Battelle Memorial Institute, to conduct the Hanford Environmental Dose Reconstruction (HEDR) Project. The DOE directive to begin project work followed a 1986 recommendation by the Hanford Health Effects Review Panel (HHERP). The HHERP was formed to consider the potential health implications of past releases of radioactive materials from the Hanford Site near Richland, Washington.

Members of a Technical Steering Panel (TSP) were selected to direct the HEDR Project work. The TSP consists of experts in the various technical fields relevant to HEDR Project work and representatives from the states of Washington, Oregon, and Idaho; Native American Tribes; and the public. The technical members on the panel were selected by the vice presidents for research at major universities in Washington and Oregon. The state representatives were selected by the respective state governments. The Native American tribes and public representatives were selected by the other panel members.

A December 1990 Memorandum of Understanding between the Secretaries of the DOE and the U.S. Department of Health and Human Services (DHHS) transferred responsibility for managing the DOE's dose reconstruction and exposure assessment studies to the DHHS. This transfer resulted in the current contract between Battelle, Pacific Northwest Laboratories and the Centers for Disease Control and Prevention, an agency of the DHHS.

The purpose of the HEDR Project is to estimate the radiation dose that individuals could have received as a result of radionuclide emissions since 1944 from the Hanford Site. A major objective of the HEDR Project is to estimate doses to the thyroid of individuals who were exposed to iodine-131. A principal pathway for many of these individuals was milk from cows that ate vegetation contaminated by iodine-131 released into the air from Hanford facilities (Napier 1992).

The HEDR Project work is conducted under several technical and administrative tasks, among which is the Atmospheric Transport Subtask. The staff on this subtask provide the daily time-integrated air concentrations and surface deposition of iodine-131 that are required to calculate doses. The atmospheric transport calculations are the link between the iodine releases estimated by the staff in the Source Terms Task and the doses calculated by the staff in the Environmental Pathways and Dose Estimates Task.

This effort includes

- development of an atmospheric model capable of describing the transport, diffusion, and deposition of material over an area of about 75,000 square miles in the vicinity of the Hanford Site

- preparation of the meteorological database required for calculation of the dispersion of material released from December 1944 through December 1949

- calculation of daily time-integrated air concentrations and surface contamination for the area and time period described above.

This report describes the atmospheric model and computer code developed by the staff of the Atmospheric Transport Task for use in these calculations. The model and implementing codes are referred to as the Regional Atmospheric Transport Code for Hanford Emissions Tracking (RATCHET). The version of RATCHET described here is the end of the model-development process that began with the MESOILT2 code (Ramsdell and Burk 1991a) and continued with development of an initial version of the RATCHET code (Ramsdell and Burk 1992). The meteorological database prepared for use with RATCHET is described by Stage et al. (1993).

This final RATCHET report is substantially different from the draft RATCHET report (Ramsdell and Burk 1992) and is, therefore, a replacement for rather than a revision of the draft report. Many of the changes in this final RATCHET report reflect changes that have been made in the RATCHET code and model parameterizations since the draft report was issued. Recent information including the results of the krypton-85 model evaluation tests and results from the model sensitivity studies have been added to the report. The source code for RATCHET and the utility codes will be published separately on a diskette rather than published as part of the report.

RATCHET has been subjected to an extensive review process. The reviewers' recommendations have been incorporated in the code and in this document but not always in a directly identifiable form because so much of the draft report was either deleted or rewritten. Therefore, the responses to the Technical Steering Panel members' comments are not being issued as part of the report but are enclosed separately with each copy.

The output from the RATCHET code has been transferred to the Environmental Pathways and Dose Estimates Task for use in dose calculations. Calculation of doses and their uncertainties were completed in late 1993. This report supersedes Ramsdell and Burk (1992) and completes Milestone 0402B.

Summary

The purpose of the Hanford Environmental Dose Reconstruction (HEDR) Project is to estimate radiation doses that individuals may have received from operations at the Hanford Site since 1944. An independent Technical Steering Panel directs the project, which is being conducted for the Centers for Disease Control and Prevention by Battelle Pacific Northwest Laboratories in Richland, Washington.

The HEDR Project modeling approach uses Monte Carlo techniques to estimate source terms, atmospheric transport, movement through environmental pathways, and dose. This approach is implemented in a suite of computer codes called the Hanford Environmental Dose Reconstruction Integrated Codes (HEDRIC). HEDRIC consists of four separate primary codes with well-defined interfaces (Ikenberry et al. 1992). The codes, which must be executed in sequence, implement

- a source-term model
- an atmospheric transport model
- an environmental pathways model
- a dose model.

This report deals specifically with the atmospheric transport model, Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET). RATCHET is a major rework of the MESOILT2 model used in the first phase of the HEDR Project; only the bookkeeping framework escaped major changes. Changes to the code include 1) significant changes in the representation of atmospheric processes and 2) incorporation of Monte Carlo methods for representing uncertainty in input data, model parameters, and coefficients. To a large extent, the revisions to the model are based on recommendations of a peer working group that met in March 1991 (Ramsdell 1992). Technical bases for other portions of the atmospheric transport model are addressed in two other documents (Ramsdell 1991; Ramsdell and Skyllingstad 1993).

This report has three major sections: a description of the model, a user's guide, and a programmer's guide. These sections discuss RATCHET from three different perspectives. The first provides a technical description of the code with emphasis on details such as the representation of the model domain, the data required by the model, and the equations used to make the model calculations. The technical description is followed by a user's guide to the model with emphasis on running the code. The user's guide contains information about the model input and output. The third section is a programmer's guide to the code. It discusses the hardware and software required to run the code. The programmer's guide also discusses program structure and each of the program elements.

The following are available on electronic media from the TSP at the address below:
1) RATCHET code, 2) code for supporting utility programs, and 3) glossary of global variables used in the RATCHET code.

Technical Steering Panel, c/o K. CharLee
Office of Nuclear Waste Management
Department of Ecology
Technical Support and Publication Information Section
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Olympia, Washington 98504-7651

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1.0 Introduction

The Hanford Environmental Dose Reconstruction (HEDR) Project is developing an integrated computer code for use in estimating radiation doses and their uncertainties. This code, called the HEDR Integrated Codes (HEDRIC) consists of four separate components (Ikenberry et al. 1992). Figure 1.1 shows the interactions of the components. The first component of HEDRIC is the Source Term Release Model (STRM) (Heeb 1993). STRM uses information about the operation of reactors and chemical processing plants at the Hanford Site to estimate hourly releases of radionuclides from the chemical processing plant stacks to the atmosphere. The second component in HEDRIC is the subject of this report, Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET). The RATCHET code combines the radionuclide release information produced by STRM with observed meteorological data and calculates daily time-integrated air concentrations and surface contamination throughout the HEDR study region. The two remaining components in HEDRIC, Dynamic EStimates of Concentrations And Radionuclides in Terrestrial EnvironmentS (DESCARTES) and Calculations of Individual Doses from Environmental Radionuclides (CIDER) (Ikenberry et al. 1992), use the time-integrated air concentrations and surface contamination data produced by RATCHET to compute annual doses.

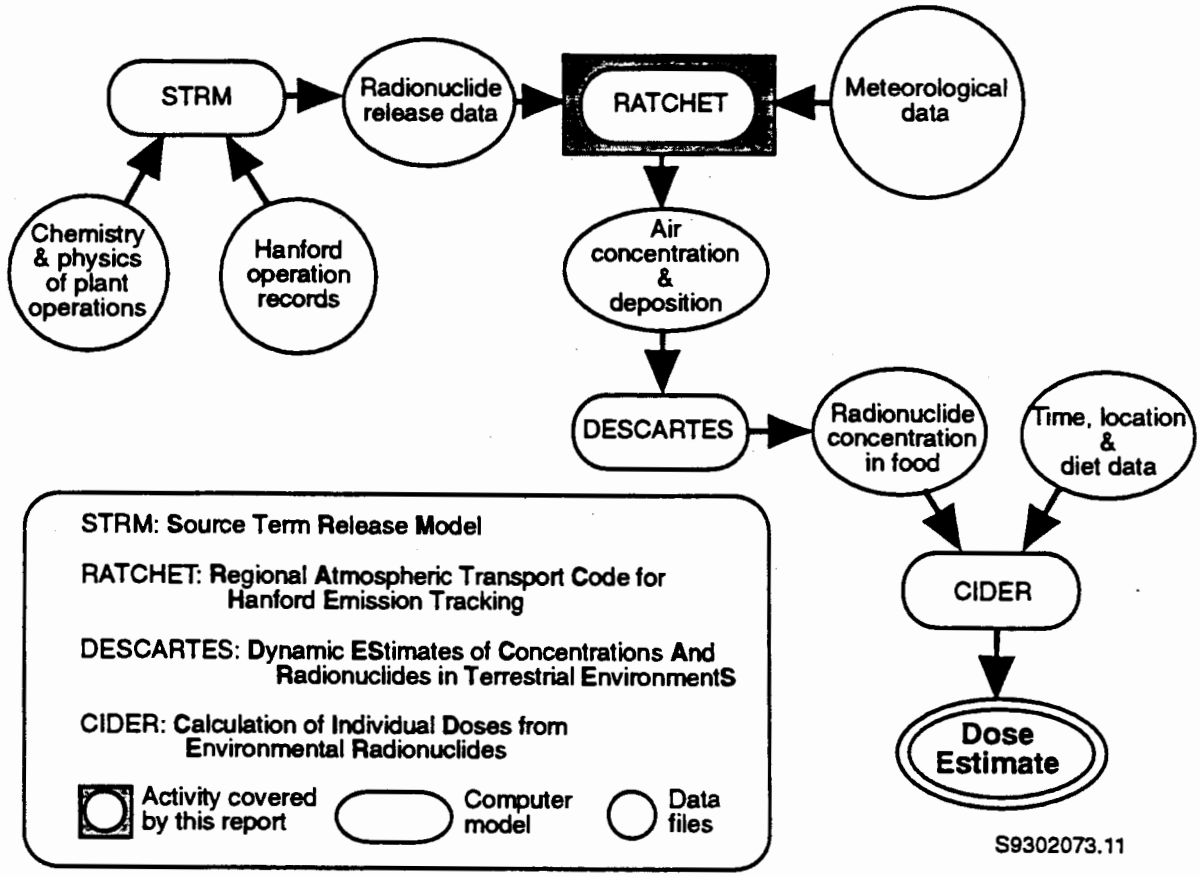

Figure 1.1. Component Interactions - HEDR Integrated Codes

1.1 Relationship to Other Atmospheric Dispersion Models

A range of atmospheric modeling alternatives for the HEDR Project was considered for the first phase of the HEDR Project (Ramsdell 1991). The recommended approach was to use a Lagrangian puff model. This recommendation was considered and accepted by the Technical Steering Panel (TSP). The MESOILT2 computer code (Ramsdell and Burk 1991a) was developed from existing code to demonstrate the technical feasibility of estimating doses from the available data. MESOILT2 is one series of codes developed from the MESODIF model developed by Start and Wendell (1974). It followed directly from the MESOI code (Ramsdell et al. 1983) and the MESORAD code (Scherpelz et al. 1986; Ramsdell et al. 1988).

The results of the initial phase of the HEDR Project demonstrated the feasibility of the puff modeling approach in that MESOILT2 provided reasonable estimates of average time-integrated air concentrations and deposition. However, the results also showed that the method of estimating uncertainty in the air concentrations and deposition needed refinement and that the spatial and temporal averaging in the initial phase masked important information (Simpson 1991a, 1991b).

After considering alternatives, a Monte Carlo approach was determined to be the only acceptable method of treating uncertainty realistically. This approach is outlined in the HEDR Project task plans for FY 1991 and subsequent years (Shipler 1991a, 1991b), which were approved by the TSP. In the Monte Carlo approach, model coefficients and parameters are varied randomly within the range of their uncertainty. The model is run many times using different coefficients and parameters in each run to obtain a range of output values. The variations in model output are examined to determine the uncertainty in the results. In the case of the HEDR Project, a model run or realization begins with the releases to the environment on December 26, 1944 and ends years later.

The representation of atmospheric processes in MESOILT2 were generally taken from models used in regulatory applications by the U.S. Nuclear Regulatory Commission and the U.S. Environmental Protection Agency. While they are accepted in regulatory applications, they do not represent the state of the science in atmospheric transport and diffusion. As a result, while the MESOILT2 code was being prepared, plans to revise the code following the calculations in the initial phase were also being developed. The decision to use Monte Carlo techniques to represent uncertainty provided additional impetus for revision and expanded the scope of the planned revision.

The revisions to MESOILT2 were so widespread that retention of the MESOILT2 name would have been misleading. Therefore, the name of the code was changed to "Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)." In this report, the name RATCHET is used in three ways. In the strictest sense, RATCHET refers specifically to the computer code discussed at length in Sections 3.0 and 4.0. In a more general sense, RATCHET refers to the code and the mathematical equations that the code implements. These equations, which model the atmosphere and atmospheric processes, are described in Section 2.0. In the most general sense in the HEDR Project, RATCHET refers to the code, the equations the code implements, and the data used as input to the code. The input data are described in various locations including Sections 2.0 and 3.0 of this report, the final meteorological database report (Stage et al. 1993), and the iodine release reports (Heeb 1993, 1994).

RATCHET is the first of a new generation of codes in the MESODIF, MESOI family. The basic framework of MESOILT2 was retained, but almost all of the representations of atmospheric processes related to diffusion and deposition have been changed. Table 1.1 compares RATCHET and

Table 1.1. Comparison of Features in RATCHET and MESOILT2

Feature	RATCHET	MESOILT2
Domain Area	~75,000 mi^2	~22,000 mi^2
Node Spacing	6 mi	5 mi
Source Term	Hourly	Monthly Average
Meteorological Data	Hourly	3-Hourly (surrogate)
Surface Roughness	Spatially Varying	None
Wind Fields	$1/r^2$ Interpolation	$1/r^2$ Interpolation
Topographic Effects	None Explicit	Empirical
Wind Profile	Diabatic	Linear
Stability	Spatially Varying, based on wind, cloudiness, and time of day... not discrete classes	Spatially Uniform, discrete classes based on ΔT at the Hanford Meteorology Station (HMS)
Precipitation	Spatially Varying, three precipitation regimes with different precipitation rate distributions	Spatially Uniform, based on HMS default rates
Mixing Layer	Spatially Varying, based on calculated values for each meteorological station	Spatially Uniform, entered with meteorological data
Plume Rise	Briggs' Equations	None
Diffusion Coefficients	Based on travel time and turbulence levels	Based on travel distance and stability class
Dry Deposition	Calculated using resistance model	Constant deposition velocity (0.01 m/s)
Wet Deposition	Reversible scavenging of gases, irreversible washout of particles	Irreversible washout of gases and particles
Iodine Representation	Partitioned between highly reactive gas, slightly reactive gas, and particles	All highly reactive gas
Uncertainty	Part of calculation	Estimated following calculation
Model Time Step	15 min maximum, 15 sec minimum	15 min maximum, 1 min minimum
Output Frequency	Daily	Monthly

MESOILT2. Most of the changes were made to ensure technical credibility and completeness of the code and to permit the code to account for uncertainty in the meteorological data. These changes were made as a group, so the effects of the individual changes have not been evaluated. In general, the net effect on dose of most of the changes should be small. However, the net effect of the changes in calculation of deposition and the treatment of iodine is to reduce the deposition by about a factor of three on and adjacent to the Hanford Site. As the distance from the Hanford Site increases, the decrease in deposition becomes less pronounced and deposition may actually increase. Two factors cause this behavior. The decrease in deposition close to the source makes more iodine available for deposition at longer distances, and the surface roughness generally increases as the distance from the Hanford Site increases. Other factors being equal, an increase in surface roughness causes an increase in deposition.

In March 1991, a working group considered representation of atmospheric processes in the transport and diffusion model. One of the group's primary concerns was the treatment of correlations among model parameters. The group's recommendations (Ramsdell 1992) include an internally consistent set of equations representing atmospheric processes. To a great extent, those recommendations were implemented in the RATCHET code. The group's recommendation related to the treatment of wind shear was not implemented because the required data are not available. This departure from the group's recommendations is discussed in detail in the wind field modeling report (Ramsdell and Skyllingstad 1993).

1.2 Quality Assurance

RATCHET has been developed in accordance with the requirements of ANSI/ASME NQA-1, 1989 edition (ASME 1989), *Quality Assurance Program Requirements for Nuclear Facilities*, as interpreted by the Battelle Quality Assurance (QA) Program. The following steps have been taken to ensure quality.

- An external workshop/peer review established the appropriate phenomena and suggested mathematical equations for RATCHET (Ramsdell 1992).
- RATCHET has been subjected to an extensive external peer review process.[(a)] Peer reviewers have included internationally recognized atmospheric scientists.
- The code has undergone extensive testing, and the test results have undergone independent review.
- An independent internal technical review of this report was performed to evaluate model implementation.
- The RATCHET code has been placed under configuration control.

(a) Letter (HEDR Project Office Document No. 09930289), "Review of the Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)," from J.E. Till (TSP) to D. B. Shipler (BNW), July 12, 1993.

The objective in the development of RATCHET was to treat atmospheric phenomena that are included in nationally accepted, applied dispersion models to the extent that available data permit. Experts outside the HEDR Project and Battelle assisted in identification and evaluation of alternative methods for estimating the transport, diffusion, and deposition to ensure completeness, representativeness, and comparability of the models implemented in RATCHET. The results of an independent review of RATCHET conducted for the Centers for Disease Control and Prevention (CDC) in early 1993 indicate that this objective has been met. Quality objectives related to RATCHET are addressed in more detail in Section 2.10.

1.3 Report Organization

The remaining sections of this report consist of a technical description of the code, a user's guide and a programmer's guide. The technical description section describes the model domain, discusses the data required by the model, and presents the equations used to make the model calculations. The technical description section also includes simple test cases that may be used to check program operation, presents the results of a model-evaluation study, and addresses data quality objectives.

The user's guide gives detailed information about the model input and output. It describes the preparation of run-specification files that are used to provide input to RATCHET and contains guidance on selecting model control parameters.

The programmer's guide provides the programming details of the code. It discusses the hardware and software required to run the code, the program structure, and each of the program elements.

The following are available on electronic media from the TSP at the address below:
1) RATCHET code, 2) code for supporting utility programs, and 3) glossary of global variables used in the RATCHET code.

Technical Steering Panel, c/o K. CharLee
Office of Nuclear Waste Management
Department of Ecology
Technical Support and Publication Information Section
P.O. Box 47651
Olympia, Washington 98504-7651

2.0 Technical Description

The RATCHET computer code implements a Lagrangian-trajectory, Gaussian-puff dispersion model. In the model, sequences of Gaussian-puffs represent plumes from ground-level and elevated sources. As the puffs move through the model domain, time-integrated air concentrations and surface contamination are calculated at locations called nodes by summing the contributions from puffs moving past the nodes. Transport, diffusion, and deposition of material in the puffs are controlled by wind, atmospheric stability, precipitation, and mixing-layer depth fields that describe the spatial and temporal variations of meteorological conditions throughout the domain.

RATCHET is diagnostic in the sense that it calculates puff movement and diffusion based on observed meteorological data. The model does not have the capability to predict changes in meteorological conditions.

This section describes the technical aspects of the atmospheric dispersion model. It first describes the model domain and coordinate systems, then continues with descriptions of the topographic and meteorological data used by the model. It then describes the source term, transport, diffusion, deposition, depletion, and decay. It discusses the treatment of uncertainty in the model. Finally, it discusses model evaluation and data quality objectives established for RATCHET.

2.1 Model Domain

The atmospheric model domain is a rectangular area. It is fixed in space and is tied to a specific location on the earth's surface by specifying the latitude and longitude for a reference point in the grid system. For the HEDR Project, the domain is centered at 46°40'N, 118°45'W, and extends approximately 306 miles from north to south and 246 miles from east to west. The HEDR atmospheric model domain is shown in Figure 2.1. The center of the model domain is offset from the release points at the Hanford Site to better fit the domain within the major topographic features of the area and to place more of the domain on the side of the Hanford Site that is downwind in the prevailing wind direction. Geographically, the domain covers an area of about 75,000 square miles that extends from central Oregon to northern Washington, and from the crest of the Cascade Mountains to the eastern edge of northern Idaho.

Wind, atmospheric stability, mixing-layer depth, and precipitation vary in time and space throughout the domain. Air temperature at the Hanford Meteorological Station (HMS) is entered as a function of time. Temperature is used in plume-rise calculations and to control scavenging of gases by frozen precipitation when the temperature is near 0°C. The spatial variation of temperature is not modeled because plume rise takes place in the immediate vicinity of HMS and because high radiation doses to the thyroid from iodine-131 tend to be associated with the milk pathway and with deposition during the summer when the temperature is well above 0°C. Section 2.7.3 discusses the relationship of temperature to wet deposition.

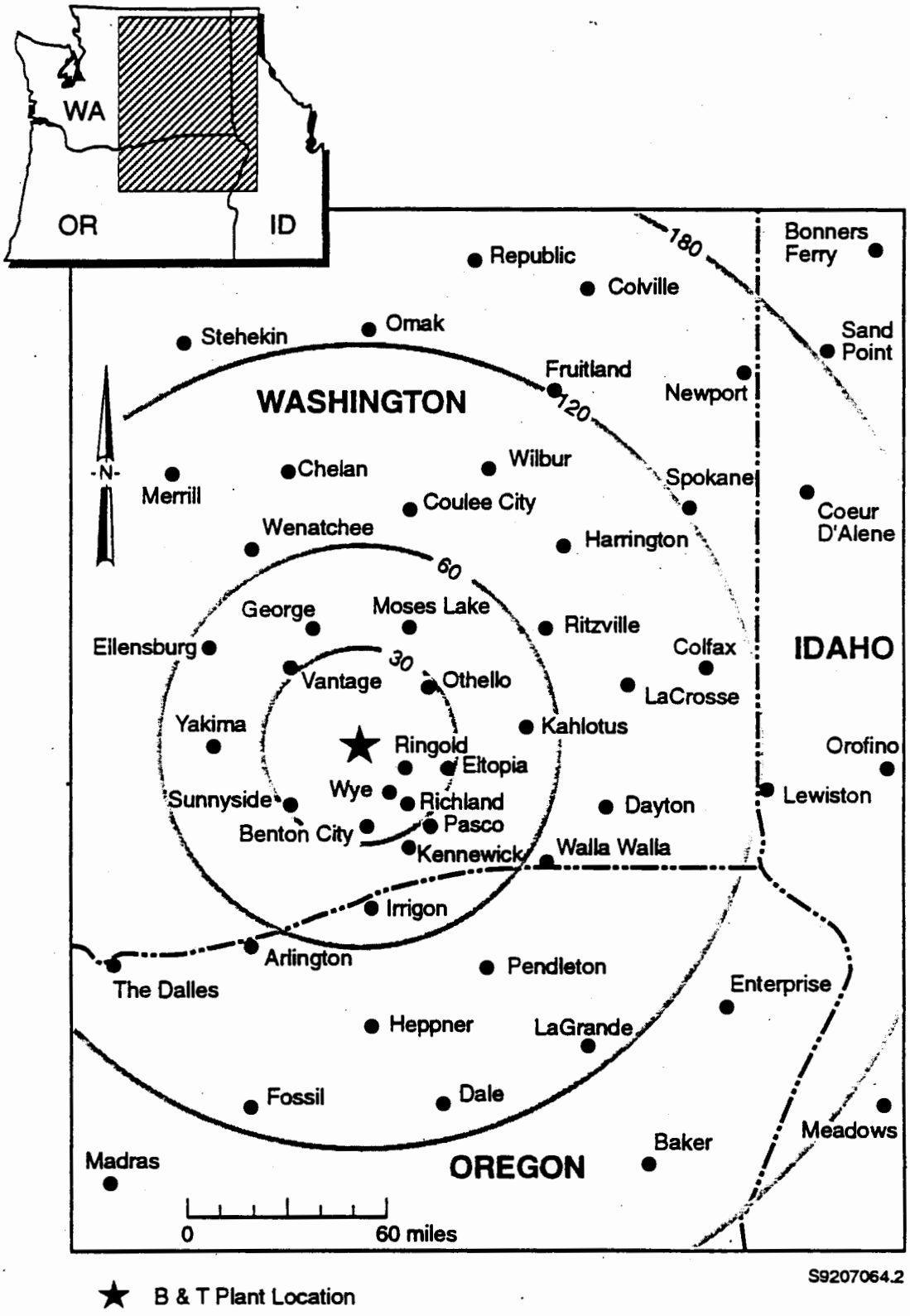

Figure 2.1. HEDR Atmospheric Model Domain

2.1.1 Cartesian Representation

Two collocated Cartesian grid systems describe horizontal positions in the domain. The first system (environmental grid) is used to specify positions and environmental conditions; the second system (concentration grid) is used for calculation of time-integrated air concentrations and surface contamination. Vertical positions in the domain are represented by height above the ground in meters.

The size of the domain is controlled by the number of nodes along the x and y axes and the spacing between nodes in the environmental grid. The concentration grid system overlies the environmental grid but has a spacing between nodes that is half the spacing between nodes in the environmental grid. Thus, a coordinate, N, in the environmental grid system has a corresponding coordinate, n, in the concentration grid system. The transformation between the coordinates is $n = 2N - 1$.

Figure 2.2 illustrates how the two grid systems are used in RATCHET. Hourly meteorological records are used to estimate the wind, stability, and precipitation at nodes on the environmental grid. These gridded values are used in the calculation of transport, diffusion, and deposition of material. As the puffs move through the model domain, the time-integrated air concentrations are calculated at nodes of the concentration grid. Finally, at the end of each simulated day, the air concentration and surface contamination grid data are written to files for use in subsequent calculations by other HEDRIC components.

The time-integrated concentrations and surface contamination calculated by RATCHET are estimates for the specific points represented by the nodes of the concentration grid. However, in the HEDRIC component computer codes that follow RATCHET, the time-integrated air concentration and surface contamination at each node are assumed to be representative for the area surrounding the node. This assumption is reasonable because the averaging time is relatively long and the points of interest are sufficiently far from the release point that the air concentration and surface-contamination gradients are generally small. The mass-balance check in RATCHET provides an indication of the accuracy of this assumption at the end of each model run.

The number of nodes along each axis is specified in PARAMETER statements in the RATCHET code. The parameters IMaxWG and JMaxWG set the number of nodes in the environmental grid; the parameters IMaxCG and JMaxCG set the number of nodes in the concentration grid. The number of nodes on the two axes do not have to be equal. The spacing between nodes on the environmental grid is specified via the run-specification file and is the same for both axes. The environmental grid for the HEDR Project has 21 nodes along the x axis, 26 nodes along the y axis, and a node spacing of 12 miles. Therefore, given the coordinate transformation above, the concentration grid has 41 nodes along the x axis, 51 nodes along the y axis, and a node spacing of 6 miles. The coordinates of the reference point are set in PARAMETER statements. The coordinates of the reference point in the environmental grid system are XRef1,YRef1, and in the concentration grid system are XRef2,YRef2. The center of the atmospheric model domain is used as the reference point for the HEDR Project.

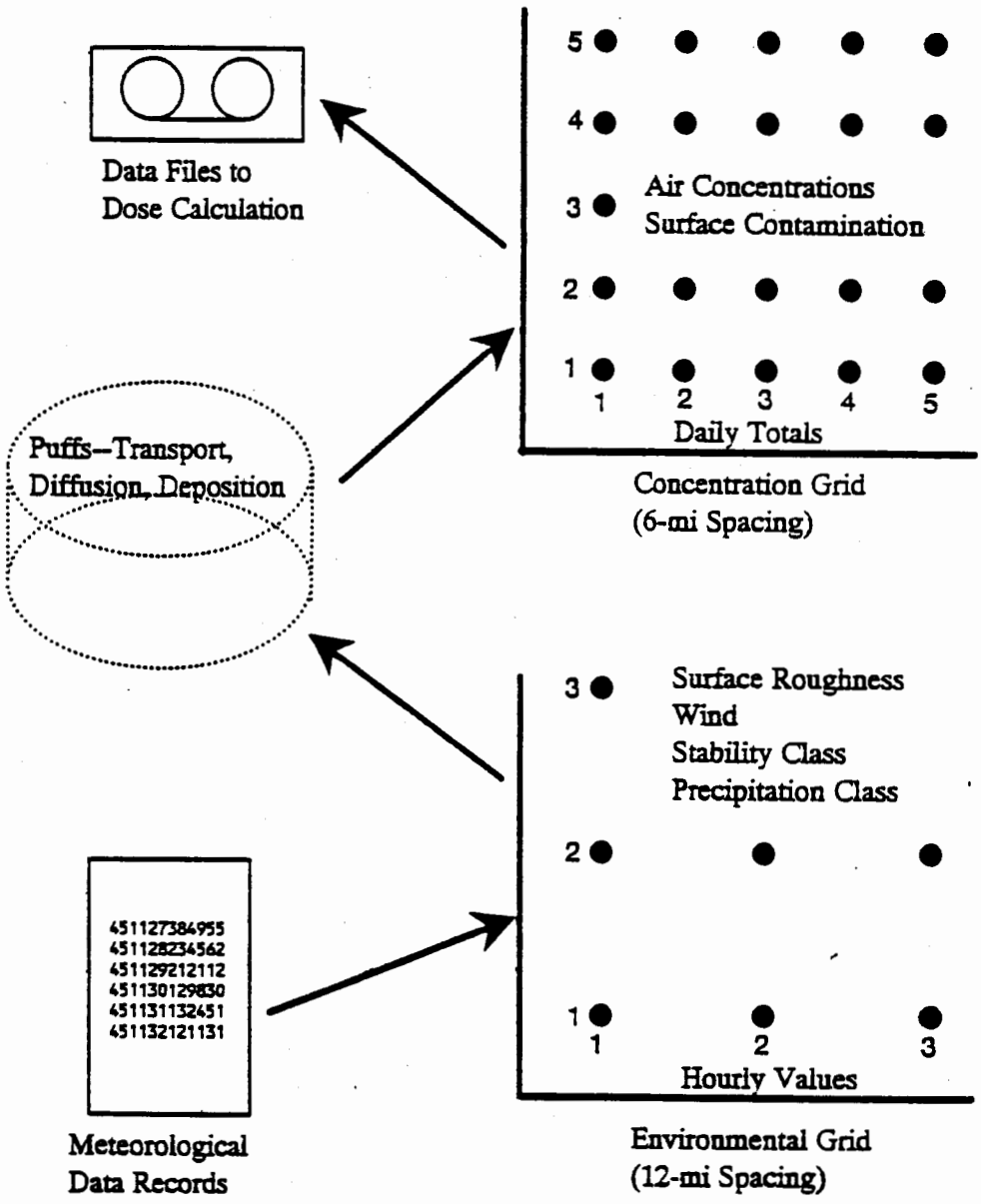

Figure 2.2. Relationship between Environmental and Concentration Grids

2.1.2 Coordinate Transformations

To facilitate association of geographic positions with model coordinates, the earth is assumed to be spherical, and a line passing through the domain reference point, parallel to the y-axis, is assumed to run north and south. With these assumptions, the standard spherical-to-Cartesian coordinate transformation can be used for converting between latitude and longitude and grid coordinates.

Expressed in finite difference form, the transformation is

$$\Delta x = r_e \cos(\phi)\, \Delta\lambda \tag{2.1}$$

and

$$\Delta y = r_e \Delta\phi \tag{2.2}$$

where Δx = east-west component of the distance between two points (km)
Δy = north-south component of the distance between two points (km)
r_e = radius of the earth ($\simeq$6370 km)
ϕ = latitude (degrees)
$\Delta\lambda$ = difference in longitude between two points (radians)
$\Delta\phi$ = difference in latitude between two points (radians).

Note that Δx is a function of latitude. The latitude of the center of the domain can be used to determine Δx for the entire domain. Although this assumption is probably adequate, a more accurate transformation was used in which all positions are referenced to the center of the grid.

Given the position of the center of the grid (x_o,y_o), and any other point x_1,y_1 with latitude ϕ_1 and longitude λ_1, then the x component of distance to the point is

$$\Delta x_1 = (x_1 - x_o) = r_e \cos(\phi_1)(\lambda_o - \lambda_1) \tag{2.3}$$

The order of the longitudes has been reversed from the usual sense so a positive Δx indicates points that are east of the center of the domain.

The center of the HEDR grid is 46.6667° N, 118.75° W. The nodes on the RATCHET output grids are 6 miles (9.656 km) apart, and node 21,26 is the center of the HEDR atmospheric model domain. With this information and equations (2.2) and (2.3), the Cartesian coordinates (I,J) on the concentration grid of a position originally given in latitude and longitude are

$$I = 21 + \Delta x/9.656 \tag{2.4}$$

and

$$J = 26 + \Delta y/9.656\ . \tag{2.5}$$

Similarly, the latitude, ϕ_n, and longitude, λ_n, of any node N(I,J) in the domain can be determined by

$$\phi_n = 46.6667 + 0.08685(J-26) \quad (2.6)$$

and

$$\lambda_n = 118.75 + 0.08685(21-I)/\cos(\phi_n) \quad (2.7)$$

where ϕ_n = latitude
λ_n = longitude
0.08685 = number of degrees of latitude between nodes.

Meteorological station locations and the positions of release points are entered as distances in kilometers along the x and y axes from the reference point. Negative distances indicate positions that are west and south of the reference location. The computer code converts distances to coordinates in the model domain using the coordinates of the reference location and node spacing for the environmental grid. The position with coordinates 1,1 lies at the southwest corner of the model domain.

The vertical extent of the model domain is unspecified. However, the atmosphere has been divided into two regions. The atmospheric boundary layer is the lower region. Its thickness is equal to the depth of the mixing layer, which varies as a function of time and location. The other region is above the mixing layer. Its depth is undefined. Within the mixing layer the wind speed and diffusion are functions of height above ground, surface roughness, and atmospheric stability. Above the mixing layer wind speed and diffusion are independent of height.

2.2 Topography

MESOILT2 (Ramsdell and Burk 1991a) included the change in terrain elevation between the positions of the center of puff and a node in the calculation of time-integrated air concentration and surface deposition at the node. This feature was included in MESOILT2 and its predecessors to account for the vertical concentration distribution in plumes passing through steep-sided valleys. The difference in elevation is not considered in the calculations in RATCHET because it would not have a significant effect on the values calculated by the code. Terrain near the release points at the Hanford Site, as resolved on the HEDR model grids, is gently sloped. Puffs rise and fall with the terrain and do not pass through any narrow valleys. At intermediate distances, vertical diffusion is sufficient to minimize the effects of differences in terrain elevation between the centers of the puffs and receptors; ground-level concentrations and deposition are nearly equal to concentrations and deposition that would be calculated assuming a ground-level release. Finally, at long range, the plume is uniformly distributed through the mixing layer, and the appropriate equations no longer include the difference in terrain elevation.

However, topography and topographic effects on transport and diffusion are not completely ignored in RATCHET. The observed wind data used in model calculations reflect the effects of the major topographic features in the model domain on transport. Wind roses in Figure 2.3 show how these effects vary across the HEDR domain. For wind roses at other locations, see Stage et al.

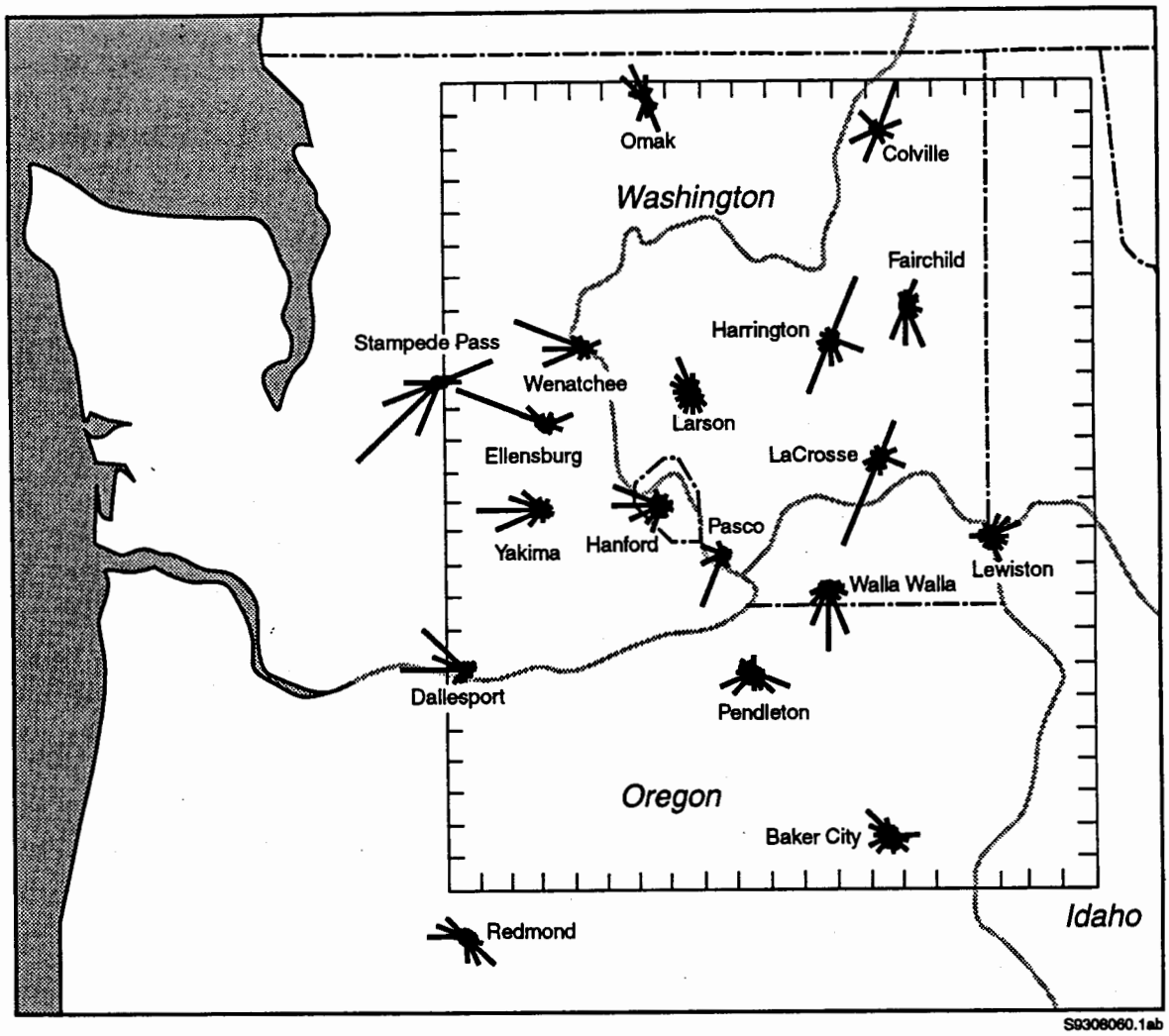

Figure 2.3. HEDR Domain Wind Roses

(1993, Figure 2.6). The prevailing wind direction for transport from the Hanford Site is shown in the wind roses for Pasco, LaCrosse, Fairchild AFB, and Felts Field. The wind roses on the western side of the atmospheric model domain show prevailing directions associated with the axes of major valleys on the eastern slopes of the Cascade Mountains. Wind roses for Pendleton and Walla Walla show contributions of the downslope flow from the Blue Mountains to the south, and the wind rose for Lewiston shows frequent flow from the Bitterroot Range to the east. The variation of winds throughout the HEDR domain is discussed in detail in the final report on the HEDR meteorological database (Stage et al. 1993).

2.2.1 Surface Roughness

The RATCHET Cartesian environmental grid is too coarse to attempt to explicitly model the effects of small-scale topographic features on puff movement. The effects of small-scale features

could not be represented accurately even if the resolution were finer because the existing meteorological data are inadequate to define these effects. RATCHET does use estimates of surface roughness (z_o), which is associated with small-scale topographic features, in modeling various aspects of the atmosphere that are directly related to transport and diffusion. These aspects include atmospheric stability, wind profiles, diffusion coefficients, and the mixing-layer depth.

A surface roughness length estimate in meters must be entered for each node on the environmental grid. The surface roughness length is a characteristic length associated with surface roughness elements. It arises as a constant of integration in derivation of the wind profile equations and is used in several other boundary-layer relationships. Texts on atmospheric diffusion and air pollution and boundary-layer meteorology (Panofsky and Dutton 1984; Stull 1988) contain tables that give approximate relationships between z_o and land use, vegetation type, and topographic roughness. Table 2.1 gives typical roughness length ranges based on data in Stull (1988, Figure 9.6).

Table 2.1. Typical Surface Roughness Lengths (Stull 1988, Figure 9.6)

Land Use/Characteristics	z_o (m)
Level grass plains	0.007 - 0.02
Farmland	0.02 - 0.1
Uncut grass, airport runways	0.02
Many trees/hedges, a few buildings	0.1 - 0.5
Average North America	0.15
Average U.S. plains	0.5
Dense forest	0.3 - 0.6
Small towns/cities without tall buildings	0.6 - 2.5
Very hilly/mountainous regions	1.5 +

Data on land use, vegetation types, and topographic roughness are readily available for the HEDR model domain. The roughness length near the 200 Areas at the Hanford Site has been determined to be in the 0.03- to 0.05-m range (Horst and Elderkin 1970; Powell 1974). Based on these results, a roughness length of 0.05 m has been assumed for the undeveloped portion of the mid-Columbia basin. Roughness lengths for the remainder of the RATCHET domain were estimated from small scale (subgrid scale) variations in ground elevations and from land use.

2.2.2 Precipitation Regimes

The spatial variation in annual precipitation within the HEDR atmospheric model domain closely follows the terrain elevations (Stage et al. 1993). This variation is due, in part, to differences in the

frequency of precipitation. However, differences in precipitation rates during precipitation periods are also important. MESOILT2 (Ramsdell and Burk 1991a) accounted for differences in the frequency of precipitation but not for differences in precipitation rates. RATCHET can account for spatial differences in both precipitation frequency and precipitation rates.

RATCHET accounts for the spatial differences in precipitation rates by allowing the user to specify three different precipitation regimes and a set of precipitation rate frequency distributions for each regime. A set of precipitation rate frequency distributions consists of six distributions—one distribution for each type of precipitation. The types of precipitation are light, moderate, and heavy rain and light, moderate, and heavy snow. The precipitation regimes and rate distributions are RATCHET input parameters in files supplied by users. Names for the files are included in the run-specification file. Details of these files are provided in Sections 3.3.2 and 3.3.3.

2.3 Meteorology

Atmospheric transport, diffusion, and deposition calculations in RATCHET are based on observed meteorological data. This section discusses the input data required by the model, adjustments to the data, and calculation of meteorological variables that were not directly measured. The final meteorological database report for the HEDR Project (Stage et al. 1993) describes the HEDR Project meteorological data in detail.

2.3.1 Meteorological Stations

RATCHET calculations require meteorological data from one or more locations. The maximum number of stations for which data can be entered is established in a parameter in the code. Routine observations are available for about 25 reporting stations in and near the HEDR atmospheric model domain during the 1940s and 1950s. Therefore, the maximum number of stations is 25 in RATCHET Version 1.2, used for the transport and dispersion calculations for this period. The maximum number of stations in RATCHET Version 1.1, which was used in the krypton-85 model-validation calculations, was 40.

The number of stations used in a specific model run is determined by the number of stations defined in a meteorological station file. The station file contains the station name and information on the station location and instrumentation. The information required by RATCHET is

- station location relative to the domain reference location (km)
- height of the wind instrument above ground (m)
- surface roughness length at the station (m)
- wind direction reporting convention (16-point compass or 10°)
- wind speed reporting units (miles per second, miles per hour, or knots)
- station status (on or off).

This meteorological station file is described in detail in Section 3.3.6.

In general, the information about meteorological stations does not change during a model run. However, over the course of the study period, some of the heights of the wind instruments changed and some of the reporting station locations were moved. A meteorological station data revision file, described in Section 3.3.7, is used for entering changes to station data. The data in the station revision file include the date of the change and the station name followed by the information listed above. Changes in station data are assumed to occur at the start of the day.

Data on meteorological station locations and wind measurement heights are contained in the station records. They are also published in the *National Wind Data Index* (Changery 1978). The convention for reporting wind direction and wind speed units should accompany the data. Prior to 1965, wind directions were generally reported in compass points. Meteorological data tapes from the National Weather Service (formerly the Weather Bureau) and other United States government agencies generally report wind speeds in knots. However, wind speeds from original station records for the mid-1940s are in miles per hour. Wind speeds for the Hanford Site are also reported in miles per hour. Wind speeds measured for use in regulatory applications are frequently reported in meters per second. RATCHET converts all wind speeds to meters per second for use in calculations.

Surface roughness lengths for stations must be estimated by the model user. Table 2.1 provides guidance in this matter.

2.3.2 Meteorological Data Input

RATCHET requires the following meteorological data:

- surface-level wind direction and speed at one or more stations
- atmospheric stability class at one or more stations
- current weather (e.g., light rain, moderate snow, etc.)
- wind direction and speed at release height
- ambient air temperature at release height.

These data are entered using the meteorological data file described in detail in Section 3.3.8. Surface-level wind data, atmospheric stability, and current weather may be entered for each station. Release height wind data and ambient air temperature are entered for the first station in the station file. The first station in station files used in the HEDR Project is HMS. Each meteorological data record is checked for missing data. When missing data are encountered for a station, the data for the hour for the station are not used in the preparation of meteorological data fields.

Each meteorological data record begins with the time of the meteorological observation. Immediately after a record is read, RATCHET determines the time of the next set of meteorological observations. The data from one observation are used until the time of the next observation. If the end of the meteorological data file is reached before the end of the simulation, the code notes that the end of the meteorological data file has been reached, assumes persistence and continues to use the last data entered. This feature facilitates preparation of meteorological data files for use in code testing. It is not used when RATCHET is run in an operational mode because meteorological data are available for the full period of interest.

Surface Wind

Wind directions and speeds are entered as two-digit integer values. The interpretation of the numerical values for each station is controlled by the codes for wind direction reporting and wind speed units entered for the station in the meteorological station file. RATCHET has provisions for entering wind directions in compass points or 10-degree increments. Wind speeds may be entered as meters per second, miles per hour, or knots.

Missing direction data may be indicated by entering a wind direction greater than 16 if directions are in compass points, or 36 if directions are in 10-degree increments. Missing wind speeds are indicated by values greater than 80. Wind speeds should be entered even if the direction is missing because they can be used in calculations of the friction velocity and mixing depth at the station.

Atmospheric Stability Class

RATCHET requires an estimate of the atmospheric stability class at each meteorological station. The stability class is entered as an integer ranging from 1 for extremely unstable atmospheric conditions to 7 for extremely stable conditions. A stability code less than 1 or greater than 7 is interpreted as missing or erroneous data.

Atmospheric stability is not observed directly. Therefore, a preprocessor program is used to estimate stability classes from meteorological data available in standard meteorological records. The preprocessor program implements a general classification scheme discussed by Pasquill (1961), Gifford (1961), and Turner (1964) for estimating atmospheric stability classes from routine meteorological measurements, including wind speed, time of day, sky cover, and ceiling height. Sky cover and ceiling height data are obtained from the hourly meteorological records.

The specific algorithm used in the preprocessor program to estimate stability class is a modified version of the National Weather Service implementation of Turner's classification scheme. The modified algorithm estimates stability if the time of day (solar altitude) and wind speed are available. Nighttime stability classes range from 6 to 4 as a function of wind speed, assuming a net radiation index of -1 in Table A-1 of Turner (1964). Daytime stability classes are determined as a function of wind speed using the unmodified insolation class number from Turner (1964, Table A-2) as the net radiation index. Additional information on sky cover, ceiling, and precipitation, as available, is used to refine stability class estimates following the complete procedure described in Turner (1964).

Current Weather

The RATCHET meteorological data record includes a code for the current weather at each meteorological station. These codes determine the precipitation type and rate used in wet deposition calculations.

The current weather code ranges from 0 to 6. A zero is used when there is no precipitation. Codes 1, 2, and 3 indicate light, moderate, and heavy liquid precipitation, respectively. Liquid precipitation includes rain, drizzle, freezing rain, and freezing drizzle. All drizzle intensities are coded as 1. Codes 4, 5, and 6 indicate light, moderate, and heavy frozen precipitation, respectively. Frozen precipitation includes snow, snow grains, snow pellets, ice pellets, ice crystals, and hail.

Release Height Wind

RATCHET uses the release height wind in plume-rise calculations. If a measurement for release height wind is available, it may be entered using the meteorological data file. Release height wind is entered in the same manner as surface winds. The wind direction convention and wind speed conversion factor specified for the first meteorological station are assumed to apply to the release height wind.

A release height wind speed greater than 80 indicates that the release height wind is not available. In this case, RATCHET uses a diabatic wind profile to estimate the release height wind using the surface wind speed, stability, and surface roughness for the first meteorological station.

Temperature

RATCHET uses the ambient air temperature at the release height in plume-rise calculations. This temperature, in degrees Celsius, is entered hourly using the meteorological data file. The code does not include a default temperature. Therefore, an ambient air temperature must be supplied in the meteorological data file, even if it is a default value. The effluent temperature, which is also used in plume-rise calculations, is input as a source term or stack variable.

In addition to its use in plume-rise calculations, the release height temperature is used to control washout of gases by frozen precipitation. In this application, the release height temperature is assumed to apply over the entire model domain.

2.3.3 Calculated Meteorological Parameters

In addition to the input for meteorological data supplied by the user, RATCHET uses several meteorological parameters that are computed hourly from the input data. This section describes the calculated parameters.

Monin-Obukhov Length (L)

Atmospheric stability classes are routinely used in dispersion modeling as a basis for choosing among alternative algorithms. However, in atmospheric boundary layer theory, a scaling length for vertical motions called the Monin-Obukhov length (L) is used as the measure of atmospheric stability. This length is needed for wind profile, turbulence and mixing-layer depth calculations.

The Monin-Obukhov length varies from a small negative value (a few meters) in extremely unstable atmospheric conditions to negative infinity as the atmospheric stability approaches neutral from unstable. In extremely stable conditions, the Monin-Obukhov length is small and positive. As neutral conditions are approached from stable conditions, the Monin-Obukhov length approaches infinity. Thus, there is a discontinuity in the Monin-Obukhov length at neutral. However this discontinuity is not a problem because the Monin-Obukhov length is found in the denominator of expressions.

Golder (1972) provides a means for converting from stability-class estimates to Monin-Obukhov lengths. Figure 2.4, derived from Golder (1972, Figure 5), shows ranges for 1/L as a function of Turner stability class and surface roughness length. Mid-range values for 1/L from this figure are used by RATCHET when a single estimate of 1/L is needed by the model.

Winds

RATCHET frequently requires wind speeds at heights other than the height at which they are measured. For example, winds at a standard height are required for wind field estimation, but historically in the United States surface-wind measurements have not been made at a standard height. Many measurements were made at about 10 meters above ground level. Therefore, RATCHET adjusts surface-wind speeds measured at heights below 8 meters and above 12 meters to 10-meter level wind speeds prior to estimating surface-wind fields. Similarly, RATCHET uses winds at puff-release height for transport calculations. Measured winds are not available at this level. Thus, RATCHET must estimate them from surface-wind data.

A diabatic wind-profile model is used to adjust wind speeds as needed. No attempt is made to model the variation of wind direction with height above ground. Diabatic profiles account for the effects of surface roughness and atmospheric stability on the variation of wind speed with height.

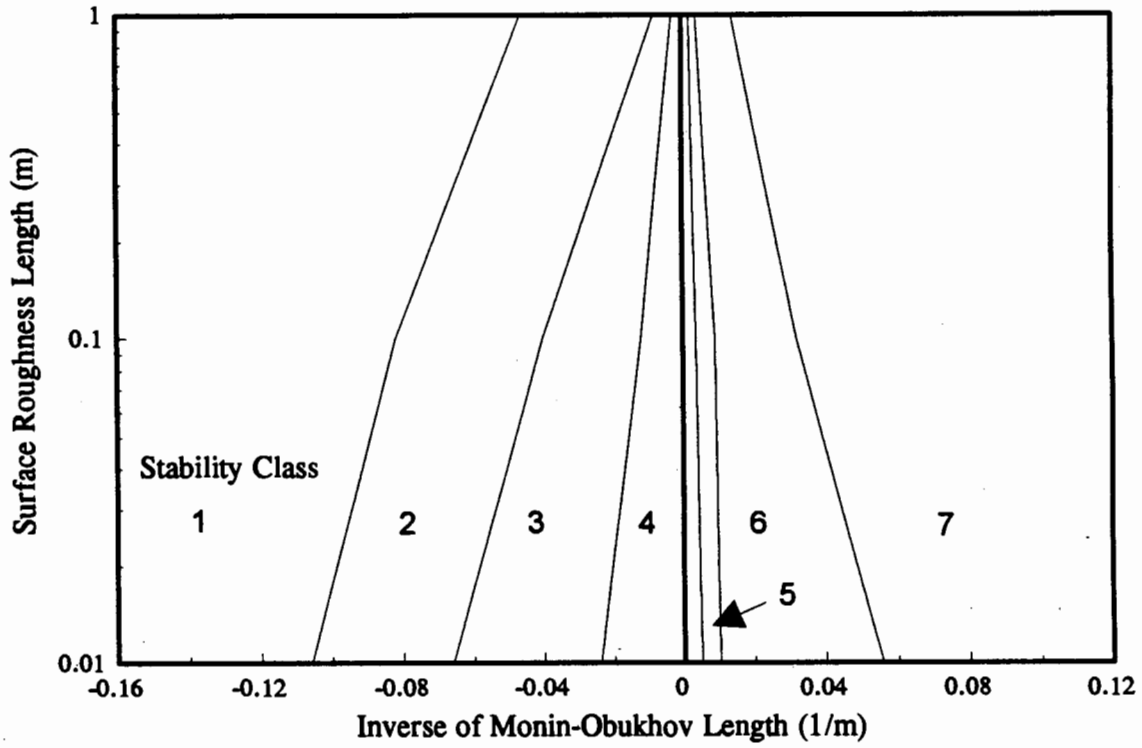

Figure 2.4. Relationship between Stability Class and Monin-Obukhov Length as a Function of Surface Roughness Length

The diabatic profile model is derived from atmospheric boundary layer similarity theory proposed by Monin and Obukhov (1954). The basic hypothesis of similarity theory is that a number of parameters in the atmospheric layer near the ground, including wind profiles, should be universal functions of the friction velocity, a length scale, and the height above ground. The length scale, L, is referred to as the Monin-Obukhov length and the ratio z/L is related to atmospheric stability. When z/L is negative and large (e.g., <-2), the atmosphere is extremely unstable (convective). When z/L is near zero, the atmosphere is neutral, and when it is positive and large (e.g., >1), the atmosphere is extremely stable. A large body of experimental data supports Monin-Obukhov similarity theory.

The diabatic wind profile is

$$U(z) = \frac{u_*}{k}[\ln(z/z_o) - \psi(z/L)] \tag{2.8}$$

where $U(z)$ = wind speed at height z (m/s)
u_* = friction velocity (boundary-layer turbulence scaling velocity) (m/s)
k = von Karman constant, which has a value of about 0.4 (dimensionless)
z = wind speed measurement height (m)
z_o = measure of local surface roughness (roughness length) (m)
ψ = stability correction factor
L = Monin-Obukhov length (m).

The term $\psi(z/L)$ accounts for the effects of stability on the wind profile. In stable atmospheric conditions, $\psi(z/L)$ has the form $-\alpha z/L$, where α has a value between 4.7 and 5.2. In neutral conditions it is zero, and the diabatic profile simplifies to a logarithmic profile.

In unstable air, $\psi(z/L)$ is more complicated. According to Panofsky and Dutton (1984), the most common form of $\psi(z/L)$ for unstable conditions is based in work by Businger et al. (1971) and Paulson (1970). It is

$$\psi(z/L) = \ln\{[(1 + x^2)/2]\,[(1 + x)/2]^2\} - 2\tan^{-1} x + \pi/2 \tag{2.9}$$

where $x = (1-16z/L)^{1/4}$. Equation (2.8) is used to estimate the friction velocity (u_*) from wind speed, surface roughness, and Monin-Obukhov length. In unstable and neutral conditions, the use of Equation (2.8) is limited to the lowest 100 meters of the atmosphere. In stable conditions, the upper limit for application of Equation (2.8) is the smaller of 100 meters or three times the Monin-Obukhov length. Skibin and Businger (1985) provide rationale for limiting application of Equation 2.8 to three times the Monin-Obukhov length in stable conditions.

Figure 2.5 shows the variation in wind speed with height between 10 and 100 meters. For unstable atmospheric conditions, the wind speed increases slowly with height, while in extremely stable conditions the increase in speed with height is relatively large. The wind speed profile for stability class 7 is only shown to a height of 70 meters because that is about the upper limit for application of Equation (2.8).

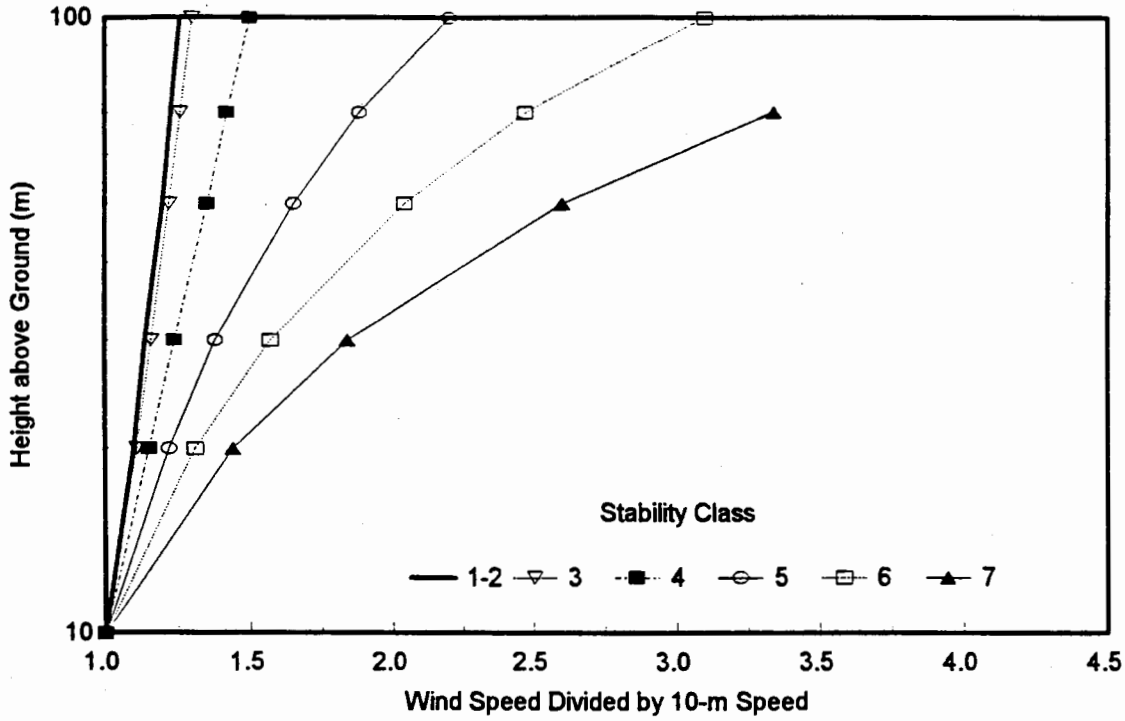

Figure 2.5. Wind Speed Variation at Heights between 10 and 100 Meters in the Diabatic Wind-Speed Profile Model

Mixing-Layer Depth

In the layer of the atmosphere next to the earth's surface, friction caused by surface roughness and heating of the surface combine to generate turbulence that efficiently mixes material released at or near the surface through the layer. This layer is referred to as the mixing layer. The top of the mixing layer is marked by a decrease in turbulence brought about by stable atmospheric conditions above. The depth of the mixing layer, also referred to as the thickness of the mixing layer, changes with atmospheric conditions. The mixing layer is generally thickest during the day and during periods with high wind speeds, and it is thinnest at night during periods with low wind speeds. In either case, the mixing-layer depth tends to increase with increasing surface roughness.

RATCHET estimates the atmospheric mixing-layer depth hourly at each meteorological station. The estimates are based on a combination of reported meteorological conditions and default values provided by the user. The choice between calculated and default values is made on the basis of the relative magnitudes of the calculated and default values, the stability, season, and time of day.

Mixing depths are calculated using relationships derived by Zilitinkevich (1972) for stable and neutral conditions. For stable atmospheric conditions, his relationship is

$$H = k(u_* L/f)^{1/2} \quad (2.10)$$

where H = mixing-layer depth (m)
k = von Karman constant (dimensionless, ~0.4)
u_* = friction velocity (m/s)
L = Monin-Obukhov length (m)
f = Coriolis parameter (s^{-1}).

Pasquill and Smith (1983) indicate that constant values in the range 0.2 to 0.7 have been suggested in place of the von Karman constant in Equation (2.10), and authors referenced by Weil (1985) suggest constant values in the range 0.4 to 0.7. RATCHET includes provisions to use either the von Karman constant or a random value selected from a uniform distribution between 0.2 to 0.7.

For neutral and unstable conditions, the mixing-layer depth is estimated using

$$H = \beta u_* / f \quad 2.11$$

where H = mixing-layer depth (m)
β = constant (dimensionless)
u_* = friction velocity (m/s)
f = Coriolis parameter (s^{-1}).

Zilitinkevich (1972) assumes that β is equal to k; Pasquill and Smith (1983) suggest β has a value in the range 0.2 to 0.3; and Panofsky and Dutton (1984) suggest its range is 0.15 to 0.25. When RATCHET is run in a deterministic mode, a value of 0.2 is assumed for β, and when run in a Monte Carlo mode, the value of β is taken from a uniform distribution between 0.15 to 0.3.

In addition to computing the mixing-layer depth, RATCHET obtains a default mixing-layer depth from a file supplied by the user. The default mixing-layer depth file is described in Section 3.3.4. It contains an array that has three dimensions with indexes based on time of day, atmospheric stability class, and month. In the default mixing-height file for the HEDR Project, the day is divided into eight 3-hour increments and the stability class index ranges from one to five (the two most unstable and the two most stable classes are combined). The data in the file are based on the hourly mixing heights estimated by the Hanford forecasters in the 5-year period from 1983 through 1987.

After a mixing-layer depth has been calculated and a default value has been obtained, the calculated and default values are compared. The larger of the two values is selected as the mixing-layer depth for the station for the hour. Ultimately, the mixing-layer height is constrained to be within the range of 10 m to 2000 m.

One additional option has been included in RATCHET. That option permits users to bypass the calculated and default mixing-layer depth and use a constant depth. This option is particularly useful when testing the code.

2.3.4 Spatial Representation of Meteorological Conditions

The RATCHET code accounts for spatial and temporal variations in atmospheric conditions between the time material is released to the atmosphere and the time it leaves the model domain. The spatial variations in the atmosphere are modeled by interpolating/extrapolating data collected at meteorological stations to nodes on the environmental Cartesian grid. The following paragraphs describe the interpolation/extrapolation methods.

Wind

Wind fields used to estimate Lagrangian trajectories for puffs are based on hourly wind speed and direction data reported for meteorological stations in and near the model domain. The wind fields are estimated by weighted averages of the reported data. Weights used are inversely proportional to the square of the distance between the station and the node. This weighting is common in spatial interpolation of wind fields (Hanna et al. 1982).

The wind fields are computed for a standard reference height of 10 m. However, puff advection is based on the winds at the effective release height. This wind is estimated by first computing the 10-meter speed beneath the puff center, then adjusting the wind speed using the diabatic wind profile model. The wind direction is not adjusted.

Ramsdell and Skyllingstad (1993) provide a detailed description and discussion of the alternatives for treating winds considered in the HEDR Project. Experimental evidence discussed in that report indicates that neither adjusting the wind fields to obtain mass consistency nor estimating upper-level winds from surface data would improve the ability of RATCHET to estimate the transport of radionuclides released to the atmosphere from Hanford operations.

Stability and Precipitation

The stability and precipitation fields are created by identifying the meteorological station with valid data closest to each node. The reported stability class and precipitation class for the station are then assigned to the node. This procedure avoids averaging that would minimize the effects of extreme stability or instability. It also permits maximum detail in treating isolated precipitation events.

Mixing-Layer Depth

Estimates of station mixing-layer depths as described above are not considered to be particularly reliable. Therefore, the spatial variation of the mixing-layer depth is modeled by fitting a plane to the estimated values using multiple linear regression (Snedecor and Cochran 1980, Chapter 17). This process provides a smooth variation of mixing-layer depth across the model domain.

When a mixing-layer depth is needed for model calculations, the regression parameters are used to estimate mixing-layer depth at the location for which it is needed. Mixing-layer depth estimates obtained from the regression are tested to ensure that they are within the range of 10 to 2000 meters. If an estimate falls outside of the range, the limiting value is substituted for the calculated value.

It is unlikely that sufficient meteorological data will be available for the regression calculations at all times or that statistically significant regression models will be obtained at all times. When there are fewer than four station mixing-layer depth estimates or the regression is not significant at the 10-percent level, a uniform mixing-layer depth is assumed. The height assumed is the average of the available estimates for station mixing-layer depths.

2.4 Source Term

RATCHET has provisions for as many as four release points. In general, the releases of concern were from B and T Separations Plants in the 200 Area at the Hanford Site. However, the model is capable of treating any release point at the Hanford Site. Each release point must be described by location, stack height (release height), stack-exit radius, nominal stack flow, and nominal effluent temperature. The number of release points and their descriptions are entered using the run-specification file.

2.4.1 Release Times and Rates

Releases from each point are treated independently from the releases at the other release points. Hourly radionuclide release rates must be provided for each release point. The release rates are contained in separate files. Names of the files are entered using the run-specification file.

2.4.2 Plume Rise and Effective Release Height

When appropriate, plume rise is computed. Although several methods exist for estimating plume rise, the equations proposed by Briggs (1969, 1975, 1984) have gained a general acceptance unequaled by the other methods. The equations that follow in this section are from the INPUFF model (Petersen and Lavdas 1986). They are implementations of Briggs' equations. Unless otherwise noted, the numerical constants in the equations are dimensionless.

Plume rise is caused by two factors, vertical momentum of the exhaust gases in a stack and buoyancy due to the density difference between the stack gases and the atmosphere. In general, one factor or the other will be dominant and the other will not contribute significantly to plume rise. RATCHET includes equations for both momentum- and buoyancy-dominated plume rise. For a given set of stack and atmospheric conditions, the temperature difference between the stack effluent and the air determines which of the factors is dominant. A critical temperature difference that separates the two regimes can be determined from the plume-rise equations. When the actual temperature difference (stack effluent temperature minus air temperature) is less than the critical temperature, momentum is the dominant factor in determining plume rise. Otherwise, plume rise is due primarily to buoyancy forces.

All plume-rise calculations in RATCHET estimate the final height of the plume. These heights are generally between 60 and 100 meters. The change in height of plumes in the vicinity of the stack is not modeled because it is several kilometers from the release points at the Hanford Site to the nearest points at which air concentration and surface contamination are computed.

In all cases, plume rise is corrected for stack downwash if the stack-exit velocity is less than 1.5 times the wind speed at the release height. The downwash correction is

$$\Delta h_d = 4r_s \, [w_p/U(h_s) - 1.5] \tag{2.12}$$

where Δh_d = downwash correction (m)
r_s = inside stack radius (m)
w_p = stack exit vertical velocity (m/s)
$U(h_s)$ = wind speed at stack height (m/s).

A minimum stack height wind speed of 1.37 meters per second is assumed when the wind is near calm (< 1.37 meters per second).

If the release height is greater than the mixing-layer height, the atmospheric stability is assumed to be extremely stable (class 7) for plume-rise calculations. Otherwise, the stability class used in plume-rise calculations is the stability-class estimate for the closest meteorological station.

Unstable and Neutral Conditions

In unstable and neutral atmospheric conditions, plume rise is dominated by momentum as long as the temperature difference between the plume and the air is less than a critical temperature difference. The critical temperature difference is calculated using

$$\Delta t_c = 0.0297 w_p^{1/3} \, T_p (2r_s)^{-2/3} \tag{2.13}$$

where Δt_c = critical temperature difference (°K)
w_p = stack exit vertical velocity (m/s)
T_p = initial plume temperature (°K)
r_s = inside stack radius (m).

Note that 0.0297 is a dimensional constant which arises from the combination of constants (and near constants) when equations 2.14, 2.15, 2.16, and 2.17 are solved for Δt_c. The specific value of the constant depends on the units used for variables in the equations. Assuming the use of metric units, the dimensions of the constant are $(m\text{-}s)^{-1/3}$.

When $T_p - T_a$ is less than Δt_c, plume rise is estimated using

$$\Delta h = 6r_s \, [w_p/U(h_s)] + \Delta h_d \tag{2.14}$$

where Δh is the final plume rise in meters and the other symbols remain as previously defined.

If $T_p - T_a$ is greater than Δt_c, the plume rise is estimated using the equation for buoyancy-dominated rise. This equation is

$$\Delta h = 1.6F_b^{1/3} x_f^{2/3} U(h_s)^{-1} + \Delta h_d \quad (2.15)$$

where F_b is a buoyancy flux parameter, x_f is the distance to final plume rise (m), and the other symbols remain as previously defined. The buoyancy flux parameter, F_b, is defined by

$$F_b = g[(T_p - T_a)/T_p] w_p r_s^2 \quad (2.16)$$

where

F_b = buoyancy flux parameter (m^4/s^3)
g = gravitational acceleration (9.8 m/s^2)
T_p = initial plume temperature (°K)
T_a = air temperature at release height (°K)
w_p = stack exit vertical velocity (m/s)
r_s = inside stack radius (m).

According to Peterson and Lavdas (1986), the distance to final plume rise, x_f, for relatively low-temperature emissions, such as those from the fuel-processing plants at the Hanford Site, is given by

$$x_f = 49F_b^{5/8} \quad (2.17)$$

The leading constant (49) in this equation has dimensions of $s^{15/8}/m^{3/2}$.

Stable Conditions

In stable atmospheric conditions, the critical temperature difference at which buoyancy-dominated plume rise exceeds momentum-dominated plume rise is

$$\Delta t_c = 0.0196 w_p T_a S^{1/2} \quad (2.18)$$

where S is a stability parameter. The dimensions of the constant in this equation are m/s^2.

The parameter S is computed from the stability class and air temperature from

$$S = gT_a^{-1} \frac{\partial \theta}{\partial z} \quad (2.19)$$

where $\partial\theta/\partial z$ is the potential temperature lapse rate. Potential temperature lapse rates of 0.02°K/m, 0.035°K/m, and 0.05°K/m are assumed for stability classes 5, 6, and 7, respectively.

When $T_p - T_a$ is less than Δt_c, momentum-dominated plume rise is estimated using Equation 2.14. It is also estimated using

$$\Delta h = 1.5S^{-1/6} [(F_o w_p T_a)/(\pi U(h_s) T_p)]^{1/3} + \Delta h_d \quad (2.20)$$

where F_o is the stack flow in m^3/s. The final estimate for plume rise is the smaller of these two values.

When $T_p - T_a$ is greater than Δt_c, one of two equations is used to estimate plume rise. If the wind speed is greater than a critical wind speed, U_c, defined by

$$U_c = 0.275 F_b^{1/4} S^{1/8} \quad (2.21)$$

then the plume rise is calculated using

$$\Delta h = 2.6 F_b^{1/3} [SU(h_s)]^{-1/3} + \Delta h_d \quad (2.22)$$

If the wind speed is less than U_c during stable conditions, the plume rise is computed using

$$\Delta h = 4 F_b^{1/4} S^{-3/8} + \Delta h_d. \quad (2.23)$$

Effective Release Height

The effective release height used for puff transport is the sum of the actual stack height and the plume rise. This height is computed in subroutine PUFFR at the time each puff is released.

2.5 Transport

There are two fundamental assumptions in all puff models. The first is that plumes can be represented by a sequence of puffs, and the second is that puff movement may be separated from puff diffusion. This section discusses how RATCHET moves puffs. The following sections discuss the calculation of diffusion and deposition.

Energy spectra computed from Eulerian wind turbulence data described by Panofsky and Dutton (1984) indicate that there is a local maximum in the energy associated with eddies with periods on the order of a few (~ 10 to 20) minutes. The spectra also indicate a minimum associated with eddies with periods on the order of an hour. Thus, there tends to be a natural division of eddy sizes in the atmosphere that roughly coincides with the observation frequency for meteorological data.

Large eddies associated with the weather systems and the diurnal variation of meteorological conditions are characterized in the hourly meteorological data. These eddies, which are treated in atmospheric transport, are large compared to the crosswind or vertical dimensions of puffs. They tend to move puffs from place to place rather than changing the size or shape of the puffs.

Hourly wind fields, based on the observed winds, are used to compute puff movement in RATCHET. However, the number of time steps used in computing puff movement is equal to the number of puffs released per hour (NPH) and is set as an input parameter in the RATCHET run-specification file. The time step used in puff movement is then 1/NPH. This interval is referred to as the puff advection period. An even shorter interval, called the sampling period is used in computing time-integrated concentrations and surface contamination. In a typical HEDR application, NPH = 4. The rationale behind this choice is discussed in Section 3.2.1.

Puff movement is computed in a five-step process. In sequence, the steps in the process are:

1. estimate the wind at puff transport height at the current puff position

2. make an initial estimate of puff position at the end of the advection period using the transport-height wind for the current puff position

3. estimate the transport-height wind at this initial estimate of the puff's position at the end of the advection period

4. using the winds estimated in Step 3 and the puff's current position, make a second estimate of the puff's position at the end of the advection period

5. average the positions estimated in steps 2 and 4.

This average position will be the position of the puff at the end of the advection period. These steps are described mathematically below.

The puff movement calculation begins by calculating the wind at the puff's current position. Bilinear interpolation is used to calculate the wind vector components at a height of 10 meters directly beneath the center of the puff from the wind vector components at the closest nodes of the environmental grid. Bilinear interpolation, which is described by Press et al. (1989), results in wind vectors that vary continuously throughout the model domain.

When the 10-m wind vector components beneath the puff center have been determined, the diabatic profile is used to adjust the wind speed to puff-transport height, if necessary. In general, the transport height for puffs will be their effective release height. The distance moved will be calculated using wind speed for the effective release height of puffs when the effective release height is ≥ 10 meters and ≤ 100 meters. The 10-meter wind speed will be used in computing movement for puffs with release heights < 10 meters, and the wind speed at 100 meters will be used to compute movement of puffs with effective release heights > 100 meters. Extrapolation of wind speeds from a height of 10 meters to heights in excess of 100 meters is not considered appropriate. The 10-meter wind direction will be used in puff movement calculations.

Next, an initial estimate of the movement is made using the components of the transport vector at the puff's starting position. For a puff initially at x,y,z, the change in position is given by

$$\Delta x = u(x,y,z)\ \Delta t$$
$$\Delta y = v(x,y,z)\ \Delta t \qquad (2.24)$$

where u and v are the east-west and north-south components of the wind vector, respectively, and Δt is the advection period (60 min/NPH). The initial estimate of the puff's position at the end of the advection period is

$$x' = x + \Delta x$$
$$y' = y + \Delta y. \qquad (2.25)$$

The transport winds at this location at the current time are then determined following the same procedure used to obtain the initial transport wind estimates. Bilinear interpolation is used to estimate the 10-meter wind components at x', y', and the diabatic profile is used to adjust the wind speed to the transport height.

The second set of estimates of the transport wind components is used to obtain a second estimate of the puff movement

$$\Delta x' = u(x',y',z)\ \Delta t$$
$$\Delta y' = v(x',y',z)\ \Delta t. \qquad (2.26)$$

Finally, the puff's position at the end of the advection period x", y" is determined from the current position and the average of the two movement estimates

$$x'' = x + (\Delta x + \Delta x')/2$$
$$y'' = y + (\Delta y + \Delta y')/2. \qquad (2.27)$$

Material in a puff continues to contribute to the time-integrated air concentrations and surface contamination at grid nodes near the edge of the model domain for a period of time after the center of the puff leaves the interior of the domain. During this period, puff movement is determined by the winds at the nearest nodes of the environmental grid. Movement is based on linear interpolation between the winds at the closest two nodes when the puff is off one of the sides of the domain, and the wind at the corner node is used when the puff is off a corner.

Movement of puffs occurs in subroutine DIFDEP and takes place in one or more steps. The number of steps is controlled by the size of the puff and the transport speed to ensure an acceptable level of precision in the calculation of time-integrated concentrations and surface contamination. The maximum number of steps that the model will take during an advection period is controlled by a parameter entered in the run-specification file. Model sensitivity to this parameter is discussed in Section 3.2.2.

2.6 Diffusion

Once material is released to the atmosphere, it acts as a passive tracer. Large-scale motions move plumes about, and small-scale atmospheric motions distribute material within plumes. The preceding discussion of transport described how RATCHET accounts for the effects of large-scale motions. This section describes how RATCHET accounts for the effects of the small-scale motions. Section 2.7 describes the deposition of material on surfaces and depletion of the puffs to account for material lost due to deposition and radioactive decay.

2.6.1 Calculation of Time-Integrated Air Concentrations

The second basic assumption in puff models is that a continuous plume can be approximated by a finite number of puffs released in succession. The concentration at a receptor is assumed to be equal to the sum of the concentrations from all of the puffs, that is

$$\chi(x,y,z,t) = \sum_{i=1}^{N} \chi_i(x,y,z,t) \tag{2.28}$$

where χ = concentration
x,y,z = position of the receptor in Cartesian coordinates
t = time of the concentration estimate
i = puff number
N = total number of puffs in the model domain.

In practice, computational rules based on puff dimensions have been established to limit the number of terms included in the summation. These rules include assigning a finite radius to each puff and combining puffs that overlap. The rules and RATCHET sensitivity to the rules are discussed in Section 3.2.

In the absence of external influences such as the ground, the concentration distribution in each of the puffs in RATCHET is assumed to be Gaussian. Diffusion in the direction of the wind and cross-wind diffusion are assumed to be equal; that is, horizontal cross sections through puffs are circular. A corollary of this assumption is that concentrations in a horizontal plane decrease as a function of increasing distance from the puff center and are independent of the direction in which the distance is increased. It is, therefore, possible to revise the definition of the coordinate system without changing the relationship in Equation (2.28). The x axis of the coordinate system now may be assumed to point toward the east, with the y axis pointing north and the vertical axis pointing upward.

Because the concentration in puffs is horizontally symmetrical, it is only necessary to know the height of the center of a puff and the distance between the center of a puff and a node to compute the puff's contribution to the concentration at the node. Therefore, the concentration distribution in puffs is defined in terms of the radial distance, r, from the puff center rather than x and y. With these assumptions, the concentration at x,y,z at time t due to puff i is given by

$$\chi_i(r,z,t) = Q(t)F(r)G(z)/[2\pi)^{3/2}\sigma_r^2\sigma_z] \quad (2.29)$$

where

- $Q(t)$ = mass of material (radionuclide) in the puff at time t
- $F(r)$ = exponential function that describes the horizontal concentration distribution
- $G(z)$ = set of terms describing the vertical concentration distribution.
- σ_r = diffusion coefficient that describes the spread of the puff in the horizontal
- σ_z = diffusion coefficient that describes the spread of the puff in the vertical

F(r) is defined by

$$F(r) = \exp[-r^2/(2\sigma_r^2)] \quad (2.30)$$

where $r^2 = (x - x_o)^2 + (y - y_o)^2$, with x,y representing the position of the node and x_o,y_o representing the horizontal position of the puff center.

The diffusion coefficient σ_r is assumed to be the same as the crosswind diffusion coefficient σ_y used in Gaussian plume models.

Definition of G(z) requires further description of the modeling assumptions. The height of the puff center above ground, which is assumed to be constant, is referred to as the effective release height. If the release is from a stack or elevated vent, the effective release height is the actual stack or vent height plus plume rise.

The ground and the top of the mixing layer are assumed to be totally reflecting surfaces for material within the mixing layer. The top of the mixing layer is not a reflecting surface for material above the mixing layer. Consequently, the top of the mixing layer is similar to a semipermeable membrane.

G(z) describes both the vertical diffusion of material and the effects of the reflection. It is an infinite sum that involves superposition of contributions from virtual sources located below the ground and above the top of the mixing layer. This approach follows from the discussion in Csanady (1973) and is described in detail in Ramsdell et al. (1983). When receptors are at ground level, as they are in RATCHET, G(z) is given by

$$G(z) = 2 \sum_{n=-\infty}^{\infty} \exp[-0.5(2nH - h_e)^2/\sigma_z^2] \quad (2.31)$$

where H is the mixing-layer depth and h_e is the effective release height.

The infinite sum of exponential terms rapidly converges to a limit. Only the terms with n = -1, 0, and 1 are used in RATCHET. When the vertical diffusion coefficient becomes sufficiently large ($\sigma_z \approx H$ or $\sigma_z \approx 0.8\ h_e$, whichever is larger), material may be assumed to be uniformly distributed in the vertical. In this case, G(z) is given by

$$G(z) = \begin{cases} (2\pi)^{1/2}\sigma_z/2H & \text{if } h_e \leq H \\ (2\pi)^{1/2}\sigma_z/2h_e & \text{if } h_e > H \end{cases} \quad (2.32)$$

and the concentration in the puff is given by

$$\chi_i(r,z,t) = Q(t)F(r)/[2\pi\sigma_r^2 H] \quad (2.33)$$

or

$$\chi_i(r,z,t) = Q(t)F(r)/[2\pi\sigma_r^2 h_e]. \quad (2.34)$$

Equation (2.33) is used when the effective release height is within the mixing layer, and Equation (2.34) is used when the release height is above the mixing layer.

Dose calculations in subsequent codes in HEDRIC require two products from RATCHET. These products are time-integrated air concentration, which is occasionally referred to as exposure, and surface contamination. Both products are output by day, with the integration periods ending at midnight. Time-integrated air concentrations, which have units of Ci-s/m^3, and the surface contamination, which has units of Ci/m^2, are computed at each node on the concentration grid covering the model domain. The spacing between nodes in this grid is set based on an entry in the run-specification file. The HEDR Project uses a concentration-grid node spacing of 6 miles.

Time-integrated air concentrations are computed from puff concentrations using the approximation

$$TIC(l,m) = \sum_{j=1}^{T/\delta t} \sum_{i=1}^{N_j} \chi_{ij}(r)\ \delta t \quad (2.35)$$

where TIC(l,m) = time-integrated concentration at node l,m (Ci-s/m^3)
j = model interval within T
T = total time period being modeled (s)
δt = duration of the time interval (60 min/NPH or less, expressed in seconds)
i = puff number
N_j = number of puffs at time interval j
$\chi_{i,j}$ = concentration at l,m due to puff i at time interval j
r = distance between l,m and the center of puff i.

The accuracy of this approximation depends upon the ratio of puff dimensions to the distance moved by the puff during the time step. Decreasing the length of the time step used in the calculation increases the accuracy of the approximation. However, it also increases computational time. Figure 2.6 shows the range of potential errors in time-integrated concentrations for an isolated plume

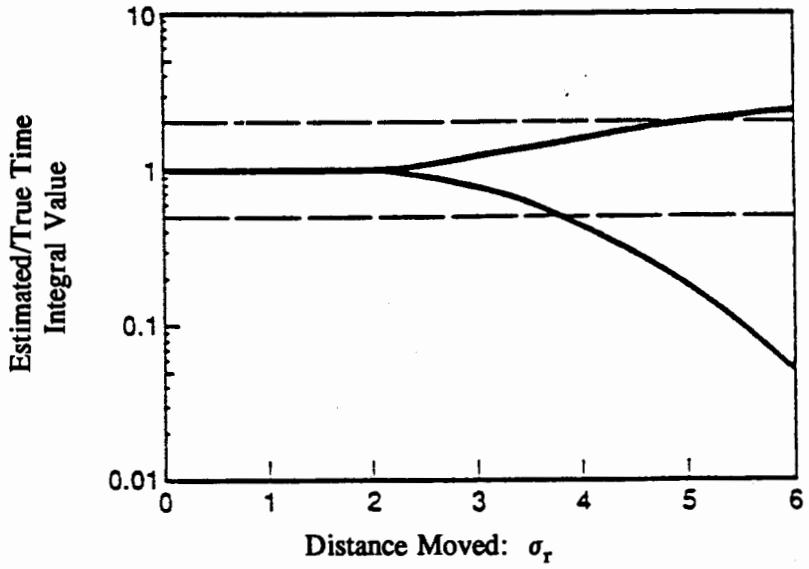

Figure 2.6. Error Band for the Numerical Procedure Used to Estimate Time-Integrated Values

as a function of the ratio between distance moved and σ_r. When the distance moved is less than $2\sigma_r$, the maximum error in time-integrated concentrations and average deposition rates is less than 10 percent. The dashed lines show that the ratio between distance moved and σ_r could be relaxed to almost four before the range of potential errors in the integrated values would increase to plus or minus a factor of two. Section 3.2.2 discusses the sensitivity of RATCHET output over periods on the order of a month to changes in the size of the minimum time step.

2.6.2 Estimation of Diffusion Coefficients

Numerous methods for estimating diffusion coefficients are described in the literature. They have been compared and evaluated by several researchers (Gifford 1976; Hanna et al. 1977; Randerson 1979; Irwin 1983; Weil 1985; Gryning et al. 1987). The general consensus is that diffusion coefficients should be estimated directly from statistics for atmospheric turbulence. Measured turbulence statistics are not available for use in the HEDR study. However, turbulence statistics may be estimated from atmospheric conditions; e.g., wind speed, atmospheric stability, and surface roughness. The estimation of turbulence statistics is discussed in the next subsection.

The diffusion coefficients included in RATCHET are for plumes because the model attempts to predict the behavior of plumes. Puff diffusion coefficients should be substituted for plume diffusion coefficients if RATCHET is used to model instantaneous (very short duration) releases.

Horizontal Diffusion Coefficients

The equation generally recommended for estimating horizontal diffusion coefficients near the source is

$$\sigma_r = \sigma_v t f_y(t) \tag{2.36}$$

where σ_r = horizontal diffusion coefficient (m)
σ_v = standard deviation of the component of the wind perpendicular to the mean direction (m/s)
t = travel time (s)
$f_y(t)$ = nondimensional function related to the travel time and turbulence time scale.

Irwin (1983) recommends that the function $f_y(t)$ be computed using

$$f_y(t) = [1 + 0.9(t/T_i)^{1/2}]^{-1} \tag{2.37}$$

where t is the travel time and T_i is the turbulence time scale, which has a value of about 1000 s.

In Equation (2.36), with $f_y(t)$ defined by Equation (2.37), σ_r increases as a function of time to the first power near the source and as a function of time to the one-half power at long times. This behavior is consistent with Taylor's (1921) theoretical result and diffusion data collected near the release point. However, Gifford (1977, 1982) presents a strong case based on both theory and observed plumes that horizontal diffusion increases at least linearly with time for several days. In addition, tests using the RATCHET code indicated that calculational results at large distances are sensitive to the minimum time step used in the model when Equations (2.36) and (2.37) are implemented in the required form. This sensitivity is not related to the diffusion calculations; it has been traced to the puff consolidation used to reduce the number of calculations. Section 3.2.3 discusses the model sensitivity to puff consolidation in more detail.

Following comments by Gifford,[(a)] a less complex algorithm for horizontal diffusion coefficients has been implemented in RATCHET. For the first hour following release, the horizontal diffusion coefficient is a function of atmospheric turbulence and time as indicated in

$$\sigma_r = 0.5\sigma_v t \tag{2.38}$$

where σ_v (m/s) is the crosswind component of turbulence and t is the travel time (s). Estimation of σ_v from available data is discussed in the next section. The value of the coefficient is the approximate value of $f_y(t)$ defined in Equation (2.37) for t = 1800 seconds (30 minutes). After the first hour, diffusion is a function of t, as shown by

$$\sigma_r = c_{sy} t \tag{2.39}$$

where c_{sy} is a proportionality constant with dimensions of meters per second.

(a) Letter (HEDR Project Office Document No. 09930289), "Review of the Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)," from J.E. Till (TSP) to D. B. Shipler (BNW), July 12, 1993.

In RATCHET, the actual calculation of σ_r is done in increments to avoid problems associated with spatial and temporal changes in conditions. The equations implemented in the code are

$$\sigma_r(t+\Delta t) = \sigma_r(t) + 0.5\sigma_v\Delta t \tag{2.40}$$

for the first hour, and

$$\sigma_r(t+\Delta t) = \sigma_r(t) + c_{sy}\Delta t \tag{2.41}$$

after the first hour. Given typical meteorological conditions, the change in algorithms at the end of the first hour generally results in an increase in the growth rate of puffs during the next several hours. This increased growth of σ_r is consistent with the growth of σ_y shown in data compiled by Gifford (1982) for travel times in the 1 to 24 hour range.

Vertical Diffusion Coefficients

The vertical diffusion coefficients may be estimated using an equation similar to Equation (2.36), with σ_z replacing σ_r, σ_w replacing σ_v, and $f_z(t)$ replacing $f_y(t)$, respectively. It is

$$\sigma_z = \sigma_w t f_z(t) \tag{2.42}$$

When this equation is applied to releases within the mixing layer, growth of σ_z is limited by the mixing-layer depth. When it is applied to releases above the mixing layer, σ_w is set to 0.01 meters per second, and σ_z is limited by the effective release height. In either case the result is that after a few minutes, σ_r is generally much larger than σ_z.

Two forms for the nondimensional function $f_z(t)$ are used by Petersen and Lavdas (1986). These are for unstable and neutral conditions

$$f_z(t) = 1 \tag{2.43}$$

and for stable conditions and above the mixing layer

$$f_z(t) = [1 + 0.9(t/T_i)^{1/2}]^{-1} \tag{2.44}$$

where $T_i = 50$ s.

Within the RATCHET code, diffusion coefficients are not computed directly from Equations (2.38), (2.39), and (2.42). They are computed from the time derivatives of these equations to permit the diffusion coefficients to properly reflect the effects of changing physical conditions. Initial diffusion coefficients are determined from the effluent flow at the release point to ensure that the concentration of radionuclides in the atmosphere is no greater than the concentration at the release

point. The diffusion rates following release depend on travel time (wind speed), atmospheric stability, surface roughness, and height of the atmospheric mixing layer. All of these factors are functions of both time and space.

2.6.3 Estimation of Turbulence Parameters

The turbulence parameters σ_v and σ_w are needed for calculation of the diffusion coefficients. These parameter are estimated as they are needed in RATCHET using atmospheric boundary layer relationships.

The relationships used in RATCHET for stable and neutral conditions are those given by Hanna et al. (1982) relating the standard deviations of the lateral and vertical components of turbulence to the friction velocity and other atmospheric boundary layer parameters. The expression for stable atmospheric conditions is

$$\sigma_v = \sigma_w = u_* \ 1.3(1 - z_p/H) \tag{2.45}$$

where z_p is the puff transport height and is below 0.9H. Above 0.9H,

$$\sigma_v = \sigma_w = 0.13u \tag{2.46}$$

For neutral conditions throughout the entire depth of the mixing layer, the expression used is

$$\sigma_v = \sigma_w = u_* \ 1.3\exp(-2fz_p/u_*) \tag{2.47}$$

Equation (2.46) is used above the mixing layer in neutral conditions.

For unstable conditions, RATCHET uses an expression given by Hanna et al. (1982) for σ_v. It is

$$\sigma_v = u_* \ (12 - 0.5H/L)^{1/3} \tag{2.48}$$

Three expressions are used to estimate σ_w in unstable conditions. If the puff transport height is in the lower half of the mixing layer, σ_w is computed from

$$\sigma_w = 1.3u_* \ (1.0 - 3.0z_p/L)^{1/3} \tag{2.49}$$

and if the effective transport height is in the upper half of the mixing layer, it is computed from

$$\sigma_w = 1.3u_* \ (1.0 - 1.5H/L)^{1/3} \qquad (2.50)$$

The first of these relationships was proposed by Panofsky et al. (1977). The second follows from the first if it is assumed that the σ_w is independent of height for z_p between 0.5H and H. Above the mixing layer it is assumed that the atmosphere is stable. Thus, σ_v and σ_w are both computed using Equation (2.36).

Ultimately, a lower bound of 0.01 m/s is used for both σ_v and σ_w. This lower bound is applied for all heights and stabilities.

The friction velocity (u_*) is computed as needed for estimating diffusion coefficients. When computed for this purpose, it is based on the wind speed, atmospheric stability, and surface roughness at the nearest node of the environmental grid. The diabatic profile relationships are used in the computation.

2.7 Transformation, Deposition, Depletion, and Decay

MESOILT2 (Ramsdell and Burk 1991a) used simple methods for calculating dry and wet deposition. The original purpose of including deposition in the MESOI family of models was to identify areas where field teams should be sent to measure surface contamination. In that context, simple deposition models were adequate. More sophisticated methods of calculating deposition have been added to RATCHET.

The model is now capable of treating four types of material—noble gases, nonreactive (slightly) gases, reactive gases, and particles. Noble gases do not deposit. The remaining types of material deposit at rates that depend on the material. Iodine is treated as a special type of material. The mass of iodine released to the atmosphere may be partitioned into nonreactive gas, reactive gas, and particulate components, and deposition is calculated using a weighted average of deposition rates.

Surface contamination is computed at nodes on the concentration grid. Spacing between nodes is 6 miles. The accumulation period for surface contamination ends at midnight each day. Material deposited on the surface is removed from the puffs to maintain a mass balance.

2.7.1 Chemical and Physical Transformation

Iodine exists in three general forms in the atmosphere. It is found in organic (slightly reactive) gases (e.g., CH_3I), in inorganic (reactive) gases (e.g., I_2), and attached to aerosol particles. These forms have significantly different deposition characteristics. For example, Voilleque and Keller (1981) give typical deposition velocities for CH_3I, I_2, and particles as 0.00001, 0.01, and 0.001 meters per second, respectively.

Burger (1991) states that the iodine should evolve from the dissolution process in the elemental form. Ludwick (1964) presents data on the change in the partitioning of iodine with distance following release of elemental iodine (I_2). In the time that it took the iodine to travel 3200 meters

(2 miles), about two-thirds of the iodine had changed form. Approximately one-third of the iodine was in organic species, and the remaining third was associated with particulate material. The partitioning of iodine at 3200 meters in Ludwick's experiments is consistent with the results of other measurements of iodine in plumes from stacks at the Hanford Site (Ludwick 1967; Perkins 1963, 1964), with the partitioning of iodine in the plume following the Chernobyl reactor accident (Aoyama et al. 1986; Bondietti and Brantley 1986; Cambray et al. 1987; Mueck 1988), and with the partitioning of natural iodine in the atmosphere (Voilleque 1979). Consequently, RATCHET assumes that the partitioning of iodine is independent of travel time.

RATCHET models the deposition of each of the three forms individually. It can also model the deposition of a mixture of the forms. Iodine partitioning is specified through three input parameters in the run-specification file. Thus, the partitioning may be changed from one model run to the next.

2.7.2 Dry Deposition

The rate of deposition of material on surfaces is proportional to the concentration of the material near the surface. The proportionality constant between the concentration in the air and the flux of material to the surface is the deposition velocity. A constant value of 0.01 meters per second was assumed for deposition of iodine-131 in MESOILT2 (Ramsdell and Burk 1991a).

The current generation of applied models estimates deposition using an analogy with electrical systems. The deposition process is assumed to be controlled by a network of resistances, and the deposition velocity is the inverse of the total resistance of the network. Resistances are associated with atmospheric conditions; physical and chemical characteristics of the material; and the physical, chemical, and biological properties of the surface. Seinfeld (1986) describes the resistance analogy.

Following the resistance analogy, the total resistance in RATCHET is made up of three components: aerodynamic resistance, surface-layer resistance, and transfer resistance. Thus, the deposition velocity is computed by

$$d_{vd} = (r_a + r_s + r_t)^{-1} \tag{2.51}$$

where d_{vd} = dry deposition velocity (m/s)
r_a = aerodynamic resistance (s/m)
r_s = surface-layer resistance (s/m)
r_t = transfer resistance (s/m).

Equation (2.51) is used in the MESOPUFF II model (Scire et al. 1984).

The aerodynamic resistance is a function of wind, atmospheric stability, and surface roughness. It is estimated as

$$r_a = U(h)/u_*^2 \quad (2.52)$$

where h is 10 meters.

The surface resistance is a function of wind and surface roughness. In RATCHET it is estimated as

$$r_s = 2.6/(0.4u_*) \quad (2.53)$$

where 2.6 is a dimensionless empirical constant and 0.4 is von Karman's constant.

Finally, transfer resistance is associated with the characteristics of the depositing material and surface type. For example, Wesley and Hicks (1977) associate transfer resistance with stomatal openings in plants. In RATCHET, the transfer resistance is used as a mathematical means of placing a lower limit on the total resistance. Users enter transfer resistance estimates using the run-specification file.

Both r_a and r_s become small as the wind speed increases. If the transfer resistance is set to zero for neutral conditions when the ratio of U/u_* is typically about 10, the dry deposition velocity computed using Equation (2.51) increases from about 0.006 meters per second for a wind speed of 1 meters per second to greater than 0.06 meters per second when the wind speed is 10 meters per second. Deposition velocities at the upper end of this range are higher than normally assumed for most reactive gases, and the entire range of deposition velocities is above the range of deposition velocities measured for fine particles ($\sim$1 micron) and nonreactive gases. Assuming transfer resistances of 10 seconds per meter for reactive gases and 100 seconds per meter for fine particles yields dry deposition velocities that are more consistent with reported values. Figure 2.7 shows the variation in deposition velocity calculated for reactive gases with wind speed and stability using Equations (2.51), (2.52), and (2.53) and a 10 seconds per meter transfer resistance. The variation in deposition velocity for fine particles shown in Figure 2.8 assumes a transfer resistance of 100 seconds per meter.

Equation (2.51) applies specifically to dry deposition of gases. It may be extended to calculation of deposition velocities for particulate material with a relatively minor modification that incorporates the gravitational settling velocity of the particles. However, as a practical matter, deposition of fine particles ($\sim$1 micron) may be estimated using Equation (2.51) because the settling velocity is small compared to the r_a^{-1} and r_s^{-1}.

Droppo et al. (1983) and Droppo (1985) published dry deposition data for ozone that include values of U and u_*. Figure 2.9 shows a comparison of deposition velocities predicted using Equations (2.51), (2.52), and (2.53), and a transfer resistance of 10 seconds per meter with Droppo's measured values. The predicted values tend to be higher than the observed values, but the correlation between predicted and observed values is as expected. McMahon and Denison (1979), Sehmel (1980), and Seinfeld (1986) all show data indicating that elemental (reactive) iodine tends to have a higher deposition velocity than ozone. Thus, the bias in the model deposition velocity estimates shown in Figure 2.9 is consistent with use of the model for prediction of reactive iodine deposition velocities.

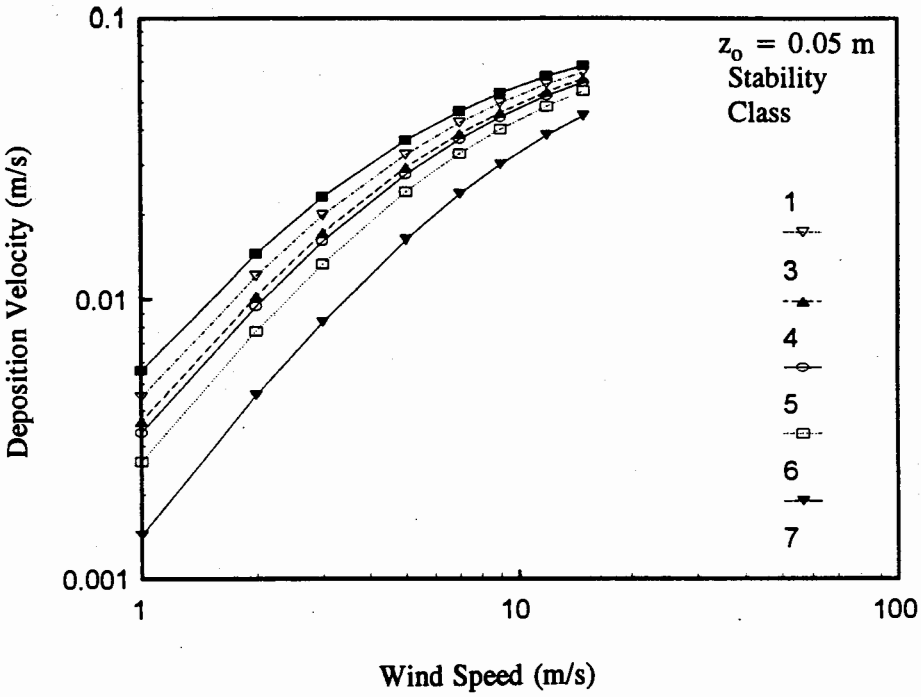

Figure 2.7. Variation of Dry Deposition Velocities for Reactive Gases as a Function of Wind Speed and Stability Class

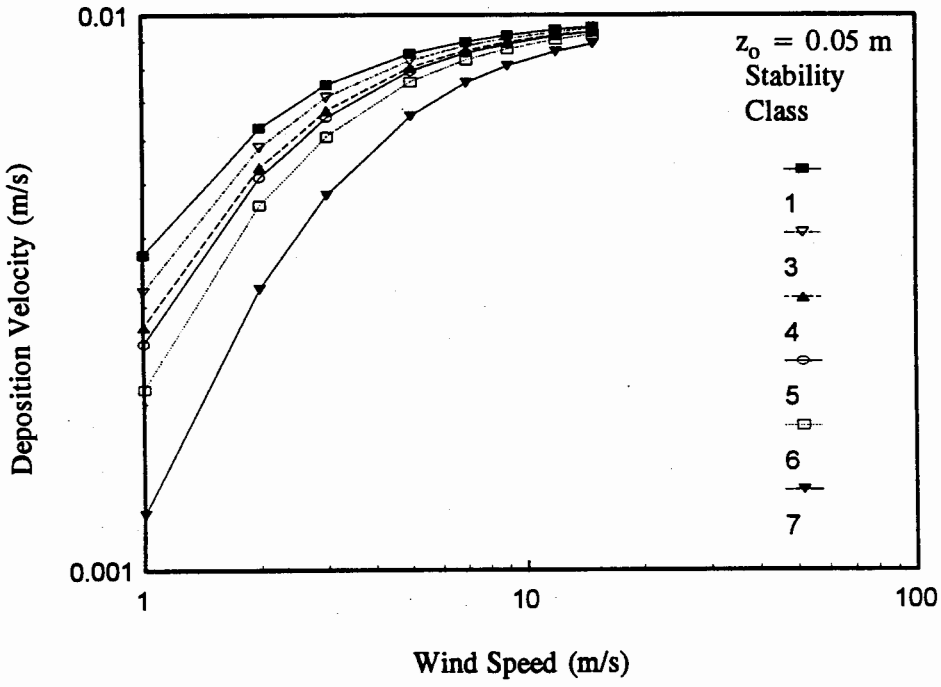

Figure 2.8. Variation of Dry Deposition Velocities for Small Particles as a Function of Wind Speed and Stability Class

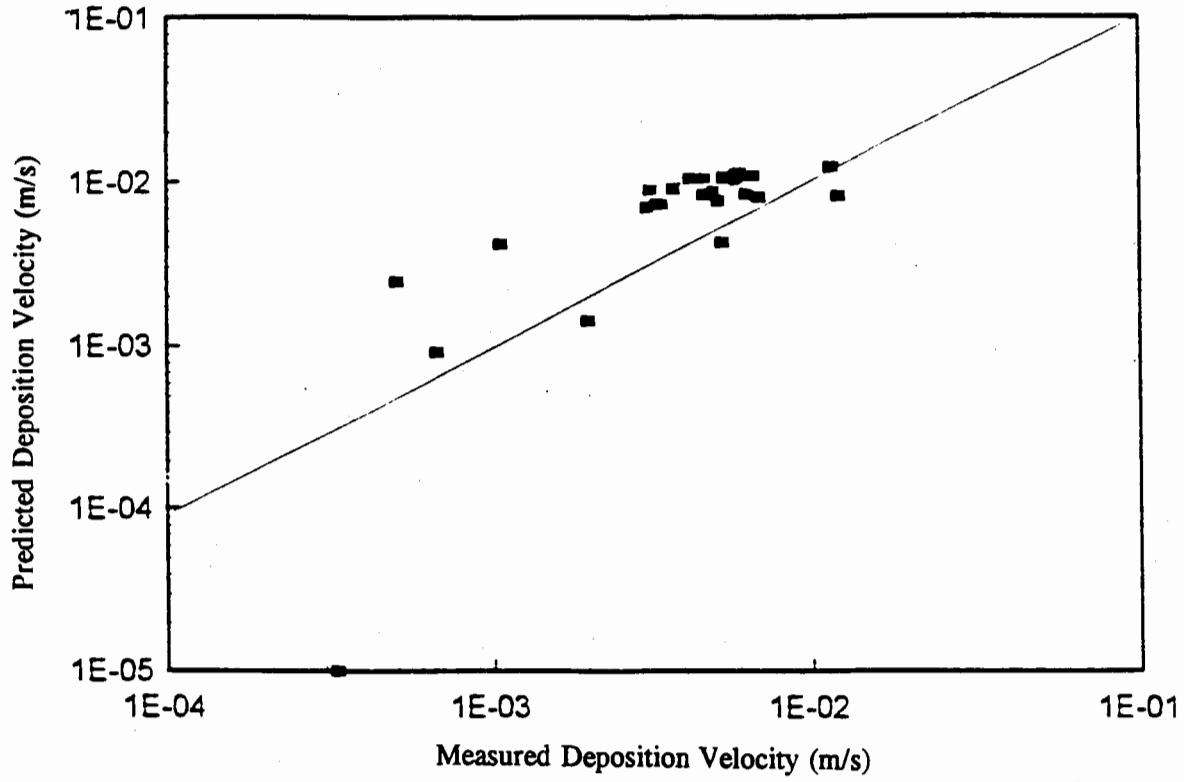

Figure 2.9. Comparison of Predicted and Measured Dry Deposition Velocities for Ozone

Separate dry deposition velocities are computed for each type of material in RATCHET. If the material exists simultaneously in more than one form, RATCHET computes a weighted-average dry deposition velocity. Such is the case with iodine. The dry deposition velocity for iodine is the weighted average of dry deposition velocities computed for nonreactive gases, reactive gases, and particles. The averaging weights for each form are based on the fraction of the iodine in the form. These fractions are input parameters entered by the user through the run-specification file. The fractions are constant during a model run, but they may be changed from one model run to the next.

2.7.3 Wet Deposition

MESOILT2 modeled wet deposition assuming washout of both gases and particles with a washout coefficient that was a coarse function of precipitation type and rate. RATCHET treats wet deposition of gases and particles separately. Wet deposition of gases is modeled assuming equilibrium between gas concentrations in the air and precipitation. Wet deposition of particles is modeled using a washout coefficient assuming irreversible collection of particles as the precipitation falls through the puffs. Slinn (1984) provides a comprehensive discussion of precipitation scavenging of particles and gases.

Scavenging rates for gases are based on solubility, assuming equilibrium conditions between the concentration of the gas in the air near the ground and in the precipitation. With this assumption, the

scavenging rate for gases is expressed as a wet deposition velocity. Slinn (1984) gives the following equation for estimating wet deposition velocities for gases:

$$d_{vw} = c\ S\ P_r \tag{2.54}$$

where d_{vw} is the wet deposition velocity, S is a solubility coefficient, P_r is the precipitation rate (water equivalent for snow) in millimeters per hour, and c is a conversion factor from millimeters per hour to meters per second.

RATCHET includes default precipitation rates of 0.1, 3 and 5 millimeters per hour for light, moderate, and heavy rain, respectively. The corresponding default precipitation rates for light, moderate, and heavy snow are 0.03, 1.5, and 3.3 millimeters per hour, respectively. These rates are consistent with hourly precipitation rates observed at the Hanford Site.

The solubility coefficients used in Equation (2.54) are inversely related to the Henry's Law constant for the gas. Users are required to enter solubility coefficients using the run-specification file. Slinn (1984) provides guidance in their selection. Assuming a solubility coefficient of 500 for reactive gases gives the wet deposition velocities shown in Table 2.2 for the default precipitation rates in RATCHET. Wet deposition velocities for nonreactive gases are about three orders of magnitude lower. If both nonreactive and reactive gases are present, RATCHET calculates a weighted-average wet deposition velocity.

Table 2.2. Typical Wet Deposition Velocities for Gases and Particle-Washout Coefficients

	Deposition Velocity (m/s)		Particle-Washout
	Reactive	Nonreactive	Coefficient (1/hr)
Light Rain	1.4 E-5	1.4 E-8	0.254
Moderate Rain	4.2 E-4	4.2 E-7	3.26
Heavy Rain	6.9 E-4	6.9 E-7	4.78

Scavenging of nonreactive gases by precipitation is extremely limited. It may be neglected by setting the appropriate solubility coefficient to zero in the run-specification file. Scavenging of both highly reactive and nonreactive gases by snow when the temperature is less than -3°C is low. RATCHET ignores scavenging of gases under these conditions.

The wet deposition model for particles assumes that precipitation falls through the full vertical extent of the puffs and collects particles by collision. The scavenging rate for particles is expressed as a washout coefficient, which is the fraction of the airborne material removed by precipitation each hour.

RATCHET uses the following expression, which is discussed in Slinn (1984), for computing washout of particles by rain:

$$\Lambda = (C\ E\ P_r)/(0.35 P_r P_n^{1/4}) \tag{2.55}$$

where Λ = washout coefficient (hr^{-1})
C = empirical constant assumed to have a value of 0.5
E = average collision efficiency assumed to be 1.0
P_r = precipitation rate (mm/hr)
P_n = normalized precipitation rate (Pr/1mm/hr).

Table 2.2 shows particle washout coefficients for the default rainfall rates in RATCHET.

During periods of snow, the washout coefficient for particles is computed using

$$\Lambda = 0.2 P_r \tag{2.56}$$

Scavenging of gases takes place when the temperature is near freezing. When the temperature falls below -3 °C scavenging ceases because of changes in the physical character of the precipitation.

2.7.4 Surface Contamination

Given the dry and wet deposition velocities, the surface contamination that accumulated at any point during a short period is computed as

$$SC1_i(x,y) = d_v\ \chi_i(x,y)\Delta t \tag{2.57}$$

where $SC1_i(x,y)$ = mass or activity deposited (Ci/m^2) at x,y from puff i
d_v = total deposition velocity, $d_{vd} + d_{vw}$ (m/s)
$\chi_i(x,y)$ = ground-level concentration (Ci/m^3) in puff i
Δt = time period (s).

Equation (2.57) simply states that surface contamination in an interval is equal to the product of a transfer coefficient (deposition velocity), the concentration in the air, and the time period.

To this contamination, RATCHET adds the contamination resulting from the washout of particles. This additional contamination is computed using

$$SC2_i(x,y) = \frac{\Lambda\ Q_i\ \exp[-0.5(r/\sigma_r)^2]\ \Delta t}{2\pi\ \sigma_r^2} \tag{2.58}$$

where $SC2_i(x,y)$ = mass deposited at x,y from puff i by washout of particles
Λ = washout coefficient (hr^{-1})
Q_i = mass in puff i
r = horizontal distance of x,y from the center of the puff
σ_r = horizontal diffusion coefficient (m)
Δt = time period (hr).

Equation (2.58) is derived by substituting a washout coefficient for the deposition velocity in Equation (2.58) and then integrating the equation from ground level through the vertical extent of the puff

The total surface contamination at x,y during any period Δt is the sum of the contributions of all puffs:

$$SC(x,y) = \sum_i [SC1_i(x,y) + SC2_i(x,y)] \tag{2.59}$$

2.7.5 Depletion

RATCHET maintains a mass balance. Material deposited on the surface by dry and wet deposition is removed from the material in the puff by decreasing the total mass of the puff. Material is not selectively removed from the bottom of the puff. This approach, which is a variation of the source-depletion model described in Hanna et al. (1982), was used in MESOILT2.

In the atmosphere, deposition results in a mass deficit in the layer of air next to the surface. Source-depletion models instantaneously propagate this deficit through the full vertical extent of the puff. This propagation is unrealistic, particularly in stable atmospheric conditions. Using the resistance analogy to estimate deposition velocities does not deal with this problem explicitly. However, using the resistance analogy results in lower deposition velocities during stable conditions, which reduces the magnitude of the error.

The mass removed from each puff is determined from analytical integration of the deposition flux over the area covered by the puff and computation interval. The mass removed from each puff to account for dry deposition of particles and dry and wet deposition of gases is computed using

$$\Delta Q_d = \Delta t \int_{\theta=0}^{2\pi} \int_{r=0}^{\infty} d_v \chi \, r \, dr \, d\theta \tag{2.60}$$

Substituting the definition of χ from Equation (2.29) for χ and performing the integration, the decrease in material becomes

$$\Delta Q_d = 2d_v QG(z)\Delta t/[2\pi)^{1/2}\sigma_z] \tag{2.61}$$

During periods of precipitation, the additional rate of mass loss from a puff by washout of particles is determined by integrating the washout rate over the area covered by the puff

$$\Delta Q_w = \Delta t \int_{\theta=0}^{2\pi} \int_{r=0}^{\infty} \frac{\Lambda QF(r)}{2\pi\sigma_r^2} \, r \, dr \, d\theta \tag{2.62}$$

When this integration is carried out, the rate of loss is equal to the product of the mass in the puff and the washout coefficient. Thus,

$$\Delta Q_w = Q[1.0 - \exp(-\Lambda\Delta t)] \tag{2.63}$$

This loss of mass is distributed throughout the puff.

RATCHET computes depletion at the end of each time step. If there is no precipitation, the mass remaining in the puff is computed assuming only dry deposition as

$$Q_{ij+1} = Q_{ij} - \Delta Q_d \tag{2.64}$$

where i is the puff index and j is a time index. When there is precipitation, the depletion calculation is

$$Q_{ij+1} = Q_{ij} \exp(-\Lambda\Delta t) - \Delta Q_d \tag{2.65}$$

2.7.6 Radioactive Decay

The atmospheric transport model accounts for radioactive decay of radionuclides with half-lives of 30 days or less. Daughter radionuclides are not considered by the atmospheric transport model. However, they are addressed in the dose models, as appropriate.

The activity of radionuclides in the atmosphere is decreased hourly to account for decay in the atmosphere. The correction for decay in the puffs is made at the end of each hour using

$$Q_{ij+1} = Q_{ij} \exp(-\lambda\Delta t) \tag{2.66}$$

where λ is the radionuclide decay constant (hr^{-1}) and Δt is 1 hour.

Deposited activity is decreased using a decay correction factor to account for decay until midnight on the day of deposition. This decay correction factor, df(t), is

$$df(t) = \exp[-\lambda(23 - t)] \tag{2.67}$$

where t is the time of day in hours at the beginning of the deposition period. The decay correction factor is applied as material is deposited if the half-life of the material is 30 days or less. Assuming the deposition in any time period is given by Equation (2.59), the surface contamination at x, y at the end of the day is calculated as

$$SC(x,y) = \sum_{j=1}^{24NPH} [SC_j(x,y)df(t)] \tag{2.68}$$

where j is a time index associated with the time of day, and the upper limit of the summation is the number of sampling periods in a day.

2.8 Uncertainty

One of the primary reasons for the extensive revision of the MESOILT2 code was to facilitate the incorporation of uncertainty in model calculations. When the number of sources of uncertainty is large and the variables in the model are correlated, a good deal of care must be taken in the way in which uncertainty is incorporated. Among the potential problems is the compounding of effects of uncertainty in an unrealistic manner.

RATCHET is basically a deterministic model. No single model run provides information on uncertainty. However, RATCHET can produce sets of results (time-integrated air concentrations and surface contamination) which, while consistent with all available data, are yet different because RATCHET includes methods for incorporating information on the uncertainty in model parameters and input data. A detailed analysis of the results of a set of model runs is necessary in order to evaluate the uncertainty in the RATCHET output.

RATCHET treats uncertainty in two ways. Uncertainties in wind direction and speed, atmospheric stability class, Monin-Obukhov length, precipitation rate, and mixing-layer height are treated explicitly within the code. Uncertainties in other model parameters such as release rates and iodine partitioning can be treated in model input. The explicit treatment of uncertainty in the variables and parameters listed above leads to the implicit treatment of uncertainty in all model calculations using these variables and parameters.

2.8.1 Random Sampling within RATCHET

RATCHET uses random sampling from specified distributions to represent the uncertainty in meteorological data and model parameters that are observed or determined external to the model. Specifically, random sampling is limited to wind directions and wind speeds, stability class, Monin-Obukhov length, precipitation rates, and station mixing-layer depths. This limitation preserves the physically based correlations among other model parameters and variables. Random sampling is controlled by the user through the run-specification file. It is selected by entering nonzero random-number seeds for those variables to be sampled randomly. The following paragraphs describe the random sampling within RATCHET by variable.

When random sampling is selected by entering random-number seeds in the run-specification file, a large number of samples is drawn in each model run. The number is sufficiently large that it is highly likely that samples will be drawn from the full range of the distribution. Therefore, simple random sampling is used within RATCHET. Simple random sampling and an alternative, stratified sampling, are discussed in the HEDR uncertainty and sensitivity analyses plan (Simpson and Ramsdell 1993).

Wind Direction

Wind direction data prior to 1965 are recorded by compass points (N, NNE,...,S,...,NNW,N). Each compass point represents a 22.5° sector. This imprecision in the recorded wind direction data is a significant source of uncertainty in atmospheric transport calculations and, therefore, in the uncertainty in concentration and dose estimates at specific points (Ramsdell and Burk 1991b). At low wind speeds, the uncertainty in wind direction is greater than the imprecision in the recorded values. There is a threshold speed below which wind instruments do not respond properly. Wind directions may be meaningless, and wind speeds are likely to be too low.

RATCHET samples from a uniform distribution to incorporate the uncertainty in wind directions because the wind direction is about as likely to be in one part of the range of uncertainty as it is to be in any other. The width of the uniform distribution is a function of wind speed. When the wind speed is reported as calm, the width of the distribution ranges from 0 to 360°. The distribution narrows as the wind speed decreases until the width of the distribution equals the imprecision in the recorded values. The method used to vary the width of the distribution in RATCHET is based on a procedure described by Schere and Coates (1992).

Other sources of uncertainty in wind directions are not considered by the random-sampling algorithm in RATCHET. These sources of uncertainty include

- one-minute observations that may not be representative of the average wind direction for the hour
- instrument exposures that may cause observed wind directions to differ systematically from the directions that are representative for the region of measurement
- changes in wind direction with height that may cause elevated plumes to move in a direction that is different from the one predicted from the reported wind direction.

Reports on wind field modeling (Ramsdell and Skyllingstad 1993) and on the HEDR meteorological database (Stage et al. 1993) describe these sources of uncertainty in more detail.

Wind Speed

Wind speeds are recorded in meteorological records in integer values in a variety of units. This imprecision in wind speeds is addressed in RATCHET. RATCHET also addresses the additional uncertainty in wind speeds near and below the instrument threshold. In general, the threshold speed of the wind instruments used in the 1940s was about 1 meter per second or 2 miles per hour.

When random sampling of winds is selected, wind speed is drawn from a uniform probability distribution because with a given wind observation there is no reason to assume that the actual speed is more or less likely to be in any part of the range of values. The width of the distribution is two reporting units when the reported wind speed is greater than 0. When a calm wind is reported, a wind speed between 0 and 2 is used if the wind is reported in miles per hour or knots. If the wind speed is reported in meters per second, a speed between 0 and 1 is used.

Wind speed measurements are subject to uncertainty from factors other than the imprecision in the recorded data and errors due to instrument threshold. This uncertainty may result from poor instrument exposure and observer bias. However, within the context of atmospheric transport and diffusion modeling, these errors may be assumed to be a minor source of uncertainty in model predictions relative to uncertainties in wind direction and stability. No attempt has been made to account for uncertainty associated with these errors.

Stability Class

Atmospheric stability is a fundamental concept in meteorology, but it cannot be calculated directly from the data available for the HEDR study period. Therefore, stability must be estimated from the limited data that are available.

Methods of estimating stability classes proposed by Gifford (1961), Pasquill (1961), and Turner (1964) are based on data that are available in routine meteorological observations. These methods form the basis of the procedure that the National Climatic Data Center uses to estimate stability classes from climatological data (Hatch 1988).

Golder (1972) compares stability-class estimates made at five locations using the method proposed by Pasquill and Turner's variation. The results of this comparison, presented in Golder (1972, Figure 3), show reasonable agreement among the hourly stability-class estimates. However, there are other studies such as the study of Luna and Church (1972) which show that these stability classes have a much wider range of uncertainty when attempting to estimate the turbulence characteristics that are related to diffusion.

RATCHET allows users to specify the uncertainty associated with stability-class estimates. This uncertainty is represented by a set of seven conditional cumulative frequency distributions—one conditional cumulative frequency distribution for each stability class. The details of the distributions are supplied by the user through a stability class uncertainty file. The name of the file is included in the run-specification file. Section 3.3.5 describes the stability class uncertainty file used in the HEDR Project.

Monin-Obukhov Length

Stability classes are discrete estimates of atmospheric stability. However, boundary-layer similarity theory uses the reciprocal of Monin-Obukhov length, 1/L, which is a continuous variable to represent stability. Figure 2.4, based on Figure 5 of Golder's (1972) paper, provides a basis for converting stability class to Monin-Obukhov length. Figure 2.4 shows the ranges of the reciprocal of the Monin-Obukhov length that is consistent with a given surface roughness length and stability class.

When random sampling of 1/L is selected by entering a random-number seed in the run-specification file, specific values of 1/L are obtained from the appropriate 1/L range as needed. The upper and lower bounds of the range are computed from surface roughness and the stability class. A random value between 0 and 1 is obtained and used to calculate a value of 1/L, assuming that 1/L is uniformly distributed within the range.

Precipitation Rates

Precipitation rates are used to compute wet deposition. Precipitation rates are not normally included in hourly meteorological observations. However, the current weather observation provides an indication of the precipitation rate at the time of observation. In RATCHET, current weather is used to determine precipitation class. If random sampling of precipitation rates is selected by entering a nonzero random-number seed in the run-specification file, precipitation rates are drawn from hourly precipitation rate cumulative frequency distributions. A precipitation rate cumulative frequency distribution is needed for each precipitation type for every precipitation region. The cumulative frequency distributions must be contained in a user-supplied file. The file name is entered through the run-specification file.

When random sampling of precipitation rate is selected, station precipitation rates are drawn from the cumulative frequency distributions for the precipitation regime in which the station is located. When precipitation fields are prepared, the precipitation rate at each node is determined by the precipitation rate at the nearest station. If the station and node are in the same regime, the rate for the station is used. If the station and node are in different regimes, an inter-regime adjustment factor is applied to the station precipitation rate to determine the node precipitation rate. With three precipitation regimes, nine inter-regime adjustment factors must be supplied by the user. These factors are entered as the last record in the precipitation rate distribution file. Details of the file are discussed in Section 3.3.3.

Mixing-Layer Depth

RATCHET computes mixing-layer depths from the friction velocity and Monin-Obukhov length. Variations in the stability class and in the computed values of the friction velocity and Monin-Obukhov length lead to variations in the computed mixing-layer depths. An additional means of varying calculated mixing-layer depths at stations has been incorporated in RATCHET. If random sampling for mixing-layer depth is selected, values for the constants k in Equation (2.10) and in Equation (2.11) are selected at random from the ranges suggested in the literature (see Section 2.3.3) assuming uniform distributions. This additional source of variability is not expected to have a significant effect on the model predictions because the model does not use the calculated mixing-layer depths in all cases. Section 2.3.3 describes the rules used to determine when the calculated values will be used.

RATCHET does not include a method for internally varying default mixing-layer depths. However, the default mixing-layer depths can be changed from one model run to the next by changing the default mixing layer file.

In general, the model output is not sensitive to uncertainty in the individual station mixing-layer depths because the station mixing-layer depths and station coordinates are used to calculate a

regression plane that describes the spatial variation of the mixing-layer depth over the model domain in an average sense. The mixing-layer depths used in model calculations are determined from the coordinates of the puff and the equation of the plane. If the regression is not significant at the 10-percent level, the average mixing-layer depth for all stations is used. In either situation, the effect of random sampling on calculation of the individual station mixing-layer depths is likely to be minimized.

2.8.2 Uncertainty Treated Externally

There are several sources of uncertainty in the model calculations that are not treated internally by RATCHET. These sources of uncertainty may be treated externally by the user if the user varies the model input from run to run. Model parameters that can be changed using input in the run specification file include:

- the proportionality constant used in calculating diffusion coefficients at travel times in excess of an hour
- the partitioning of effluent among different species
- the transfer resistances used in calculating dry deposition velocities
- the solubility coefficients used in calculating wet deposition velocities of gases
- the stack parameters used in calculating plume rise.

In addition, users may vary the information in files used to define source terms, surface roughness length fields, and default mixing-layer depth to account for uncertainty.

When uncertainty is treated externally, the number of samples drawn from the distribution describing the uncertainty is relatively small. Consequently, a stratified sampling procedure should be used to ensure that samples are drawn from the full range of the distribution. In stratified sampling, the range of the distribution is subdivided into regions of equal probability and an equal number of samples is drawn from each region. Stratified sampling was used in the HEDR Project to select the diffusion coefficient proportionality constant and the effluent partitioning coefficients; the other parameters were not varied.

Treating the source-term uncertainty externally is essential in the HEDR Project because it is the only way of applying realistic physical constraints to the release times and magnitudes in the source-term time series. If the source-term time series were to be generated within the atmospheric model, random sampling of release times and rates could lead to unrealistic release scenarios. For example, if release rates early in a run segment are too low, unrealistically high release rates might be required at the end of the segment to match a known monthly total release.

In the HEDR Project, source-term uncertainty is treated using a set of 100 realizations of release rates and times generated by the HEDR source-term model. Each realization of the complete source-term time series is based on and consistent with available reactor and fuel-processing plant records.

When RATCHET uses a different realization of source-term time sequence in each model run, the variability in atmospheric model output reflects the uncertainty in both the source-term and atmospheric models.

2.9 RATCHET Model Evaluation

Napier et al. (1993) describe the model-validation plan for the Hanford Environmental Dose Integrated Codes (HEDRIC), which include RATCHET. The plan describes the general strategy for model validation. This strategy includes four steps. These steps are:

- peer review of the models during model development
- verification of the computer implementation of the models
- verification of the assumptions and parameters in the codes
- comparison of code predictions with measurements.

Experts in description of the atmospheric boundary layer and in transport and diffusion have been involved in the development of the RATCHET code (Ramsdell 1992). Other experts acted as peer reviewers during development. A third set of experts reviewed the code and preliminary documentation for the CDC.[(a)] These reviews have addressed the models, parameters, and assumptions in RATCHET. The RATCHET code has undergone extensive developer tests. These tests checked individual program elements (subroutines and functions) and integration of the elements within RATCHET. An independent review of the code was conducted following completion of the developer's tests.

The HEDR model-validation plan describes eight sets of monitoring data used to validate the models in HEDRIC, including RATCHET. The measured data in seven of the eight data sets are iodine-131 concentrations in vegetation or iodine-131 thyroid or body burdens. In these cases, comparisons of model predictions with measured data provide information on the performance of a sequence of models without providing information on the specific models in the sequence. The results of these comparisons are presented by Napier et al (1994).

The eighth data set is a set of measurements of krypton-85 made between November 1983 and September 1987 at 10 locations on the perimeter of the Hanford Site and in nearby communities. These data may be compared directly with RATCHET output. This section focuses on the comparison of RATCHET predictions with krypton-85 measurements.

2.9.1 Krypton-85 Monitoring Data

The krypton-85 monitoring program was in place when the PUREX plant, which is a major source of krypton-85, was restarted in 1983. The monitoring program collected air samples by slowly pumping about 0.3 m^3 of air into a bag over a 4-week period. Following sample collection, the krypton was cryogenically separated from the rest of the sample and counted in a low-temperature

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(a) Letter (HEDR Project Office Document No. 09930289), "Review of the Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)," from J.E. Till (TSP) to D. B. Shipler (BNW), July 12, 1993.

liquid scintillation counter with a detection limit of about 2 pCi/m^3. For samples above background, the $\pm 2\sigma$ counting error is about 10 percent of the measured value (Woodruff 1988).

Table 2.3 lists the krypton-85 monitoring locations, their positions relative to the PUREX plant, the time period during which the samples were collected, and the number of samples collected. Two air samplers were located at the 300 Area Trench on the north side of the 300 Area. Occasionally, the samplers were operated simultaneously. The data from the periods of simultaneous operation provide a second means of estimating uncertainties in the krypton-85 data. Figure 2.10 shows a comparison of krypton-85 concentrations measured by the two samplers. In general, there is good correlation between the measured values. Despite the good correlation and the small counting error, differences of the order of a factor of two do occur. Nevertheless, the quality of these data is better than can be expected for other data sets used in validation.

The krypton-85 data provide an opportunity to evaluate RATCHET's ability to predict monthly time-integrated air concentrations for a nondepositing material. Neither the measured nor the predicted concentrations are affected by deposition. The concentrations are a function of the release rate and timing, atmospheric transport, and diffusion. Based on analysis of krypton-85 data, errors in RATCHET deposition calculations and in subsequent HEDRIC model components will not affect model evaluation.

Table 2.3. Krypton-85 Monitoring Station Data

Monitoring Location	Bearing/Distance from PUREX (deg)/(km)	Monitoring Period	Number of Samples
300 Area Trench	136/26	1983-1987	42
		1983-1987	25
Fir Road	120/24	1984-1987	34
Prosser Barricade	154/19	1984-1987	28
Ringold	090/22	1983-1987	40
Sagehill	054/24	1984-1987	32
Pasco	136/46	1986-1987	22
Eltopia	105/40	1986-1987	15
Othello	043/41	1986-1987	18
Sunnyside	234/43	1984-1987	41
Yakima	272/77	1986-1987	18

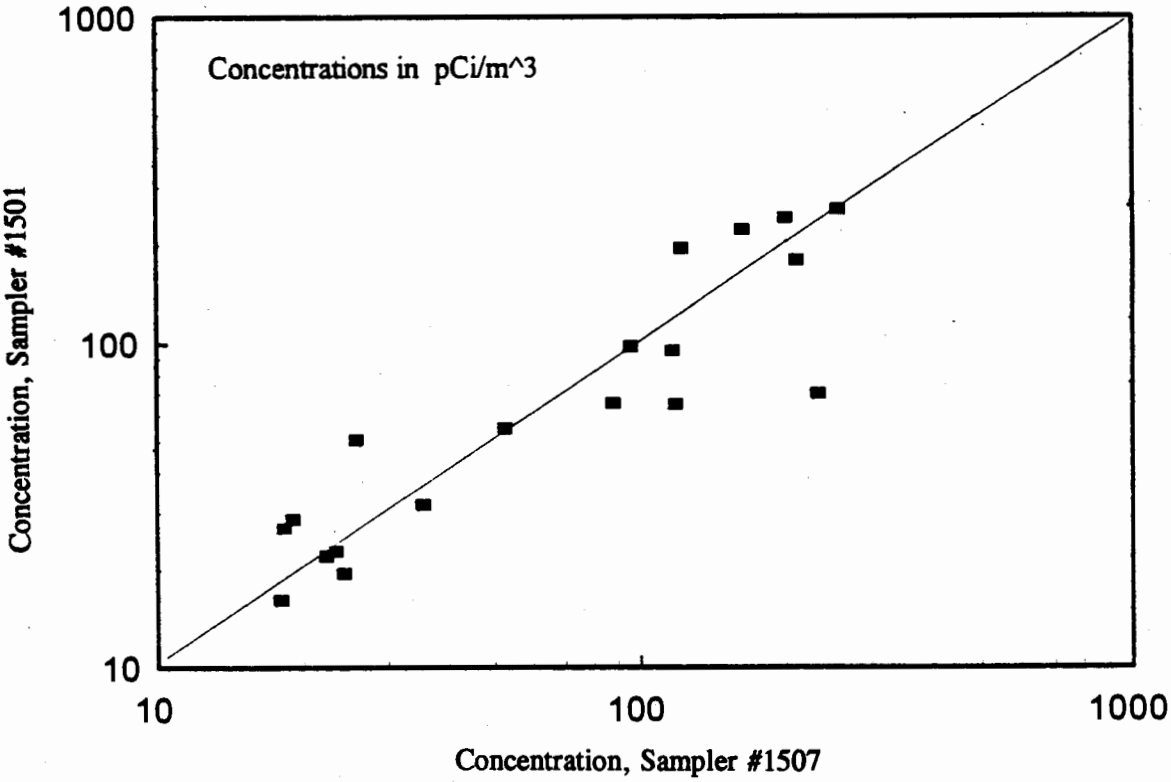

Figure 2.10. Comparison of Krypton-85 Concentrations in Samples Collected by Two Different Air Samplers at the Same Location

2.9.2 Krypton-85 Source Term

The environmental monitoring reports for 1983 through 1987 (Price et al. 1984; Price et al. 1985; Price 1986; PNL 1987; Jaquish and Mitchell 1988) list the annual releases of krypton-85 by area from the Hanford Site. These reports indicate that the 200 Area (PUREX separations plant) released approximately 1,690,000 curies of krypton-85 during this period. The PUREX plant releases overwhelmed releases from any other location at the Hanford Site. The only other krypton-85 releases mentioned in these reports were 350 curies released from the 400 Area (Fast Flux Test Facility) in 1985 and 45,000 curies released from the 100 Area (N Reactor) in 1986.

PUREX plant processing records provide sufficient information to reconstruct approximate hourly release rates from November 1983 through September 1987. These records included

- fuel charged into the dissolvers (dates and amounts)
- periods of dissolution (number, time, and duration) by dissolver
- total amount of fuel dissolved each month.

The following assumptions were made in converting this information and the total number of curies of krypton-85 released from PUREX each year to hourly release rates:

- the number of curies of krypton-85 released per hour was constant during dissolution
- the krypton-85 hourly release rate from PUREX was equal to the sum of the release rates computed for the active dissolvers
- the number of curies of krypton-85 released per ton of fuel processed was constant during a year.

Figure 2.11 shows the monthly totals of the krypton-85 releases estimated with these assumptions. Hourly release rates within each month were highly variable because the dissolution of reactor fuel is a batch process and the number of dissolvers in operation at any time ranged from zero to three. Typically, dissolution lasted for about 12 hours.

The hourly krypton-85 release rates estimated for use in RATCHET evaluation do not account for the uncertainty inherent in the estimates. The variability in RATCHET concentration estimates will be underestimated because this uncertainty has not been addressed in model calculations. The assumptions used to generate the hourly release rate estimates are clearly sources of errors, and the errors may not be random. The effect of errors associated with the assumption that the rate of release

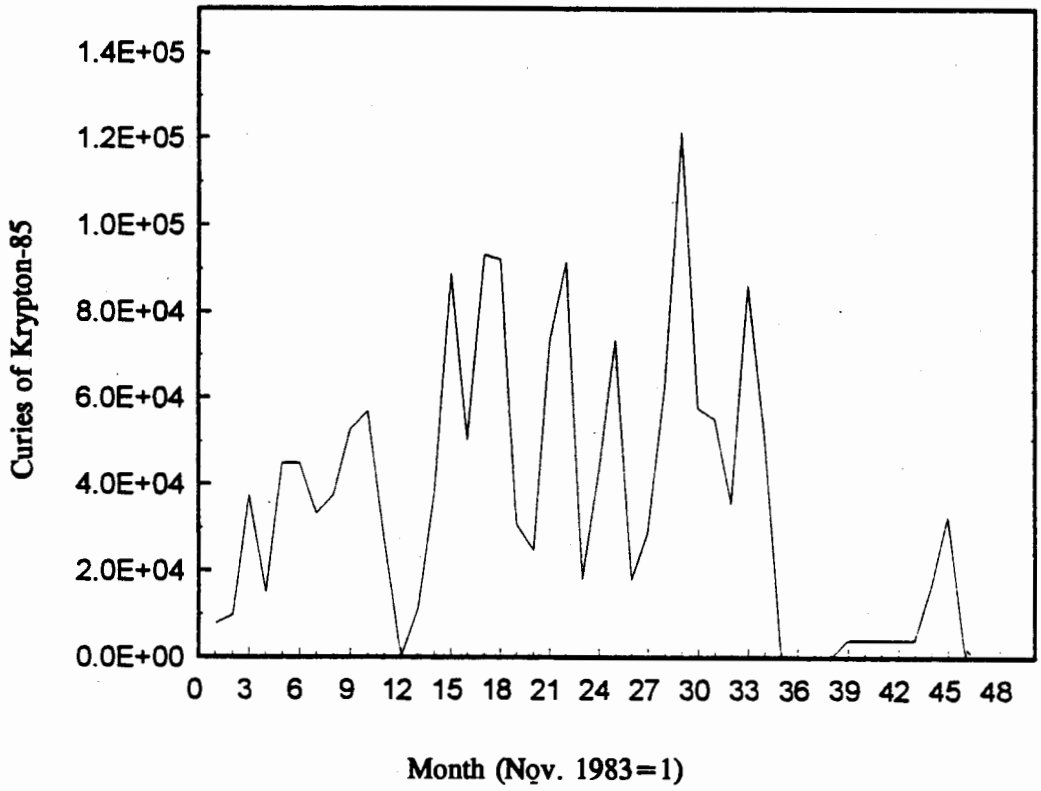

Figure 2.11. Monthly Krypton-85 Releases from the PUREX Plant, November 1983 - September 1987

of krypton-85 is constant during dissolution is likely to be minimized by the long sample collection period. Similarly, the effect of errors in estimates of the time and duration of dissolution periods may be minimized by the averaging done in sample collection. In contrast, the assumption that the curies of krypton-85 released per ton of fuel processed is constant throughout a year may not be minimized by the sample collection.

2.9.3 Meteorological Data

Meteorological data for 1983 through 1987 used for the earlier HEDR calculations (Ramsdell and Burk 1991b) were used to calculate krypton-85 concentrations for comparison with the krypton-85 monitoring data. These data consist of the meteorological observations at HMS and 12 other regular weather observation stations in and near the model domain. The meteorological data also include wind directions and speeds for 25 surface stations on and adjacent to the Hanford Site that comprise the Hanford Telemetry Network.

Data for six of the telemetry stations near the PUREX Plant were not used in order to ensure that the wind at the 200-foot level of the HMS tower received proper weight in determining the wind field in the vicinity of the release point. Data from two other stations (Rattlesnake Mountain and Gable Mountain) were not used because they are more representative of winds aloft than they are of winds near the surface.

All of the wind directions for this period are reported in 10-degree increments. This resolution is better than the wind direction resolution in the meteorological data set used by RATCHET in other HEDR calculations. No attempt was made to degrade the wind direction resolution to match that in the other data sets.

2.9.4 RATCHET Computer Runs

Version 1.1 of the RATCHET code was used for model calculations for comparison with the krypton-85 data set. There is no difference in the atmospheric transport and diffusion calculations between RATCHET Version 1.1 and the code documented in this report. The two primary differences between the versions are 1) the maximum number of meteorological stations in Version 1.1 is 40 rather than 25, and 2) Version 1.1 includes an additional output subroutine to create a file containing the daily time-integrated concentrations for 20 nodes that are in the vicinity of the monitoring locations.

RATCHET was run using the option that skips calculation of deposition because krypton is a noble gas. The half-life was set to zero to bypass the radioactive decay calculations. Krypton-85 has a half-life of 10.7 years. Therefore, neglecting decay in the model calculations does not affect the concentrations significantly.

Two sets of RATCHET runs were made for comparison with the krypton-85 data. The first set consisted of 50 runs using the full meteorological data set with the exceptions noted above. The second set consisted of 50 runs using meteorological data from only those stations that were available for other HEDR calculations. The first set of model runs was made to provide data for use in

evaluating the RATCHET model. The second (limited) set was made to provide data for use in evaluating RATCHET within the HEDR meteorological data environment.

Following completion of the RATCHET calculations, the files containing the data for the nodes in the vicinity of monitoring locations were transferred to a personal computer. A utility program then simulated the monitors by accumulating the daily, time-integrated air concentrations at the node nearest each monitoring location for periods when an air sampler was active.

It was assumed that all sampling periods started and ended at noon. Thus, only one half of the daily value was added to a sample on the first and last days of the sampling period. The utility program then 1) converted the sample to concentration by dividing by the duration of the sample collection period, 2) converted the concentration units to pCi/m^3, and 3) added a background concentration of 24 pCi/m^3 to the calculated value because RATCHET does not consider the background. The alternative to adding background to the calculated concentrations would be to subtract the background from measured concentrations. However, this results in negative concentrations and small concentrations that may or may not be background.

The background concentration was estimated from air sampling data collected during periods when Hanford operations were not releasing krypton-85. The background data are summarized in Table 2.4. These data do not show a significant variation in the background between 1983 and 1987, although increases in the local and global background of krypton-85 have been noted (Woodruff et al. 1991). Besides the absence of a temporal trend, there does not appear to be any systematic spatial variability in the background data.

Table 2.4. Krypton-85 Background Concentration in the Vicinity of the Hanford Site, 1983-1987

Monitoring Location	Number of Samples	Average Background (pCi/m^3)	Standard Deviation (pCi/m^3)
300 Area Trench	11	21.9	5.6
	18	22.8	4.3
Fir Road	8	26.4	6.1
Prosser Barricade	5	23.3	4.4
Ringold	8	22.7	4.3
Sagehill	9	24.9	4.5
Pasco	8	26.6	8.4
Eltopia	7	25.1	4.3
Othello	8	23.0	4.2
Sunnyside	14	20.0	4.8
Yakima	8	24.0	3.8
TOTAL	104	23.35	5.43

2.9.5 Node 17,23 Time Series

Air samples were simulated from RATCHET output by accumulating the daily, time-integrated air concentrations at nodes for periods corresponding to the times of sample collection, typically 28 days. Each sampler was assumed to be at the location of the nearest node. No attempt was made to interpolate time-integrated concentrations from the nodes to the actual sampling locations. As a result of this process, three samplers were assumed to be located at node 17,23 of the RATCHET/ HEDR concentration grid. Node 17,23 corresponds to a location in the middle of the Columbia River approximately midway between the 300 Area Trench and Fir Road sampling locations.

The data for these three samplers provide an almost continuous record of krypton-85 concentration in the vicinity of node 17,23 from November 1983 through September 1987. In addition, there are many periods within this time frame when there was more than one sampler in operation. As a result, node 17,23 is an ideal location for comparison of RATCHET concentration predictions with measured data.

Figure 2.12 compares the median concentration predicted by RATCHET for node 17,23 in model runs with the full meteorological data set with the krypton-85 concentrations measured at the

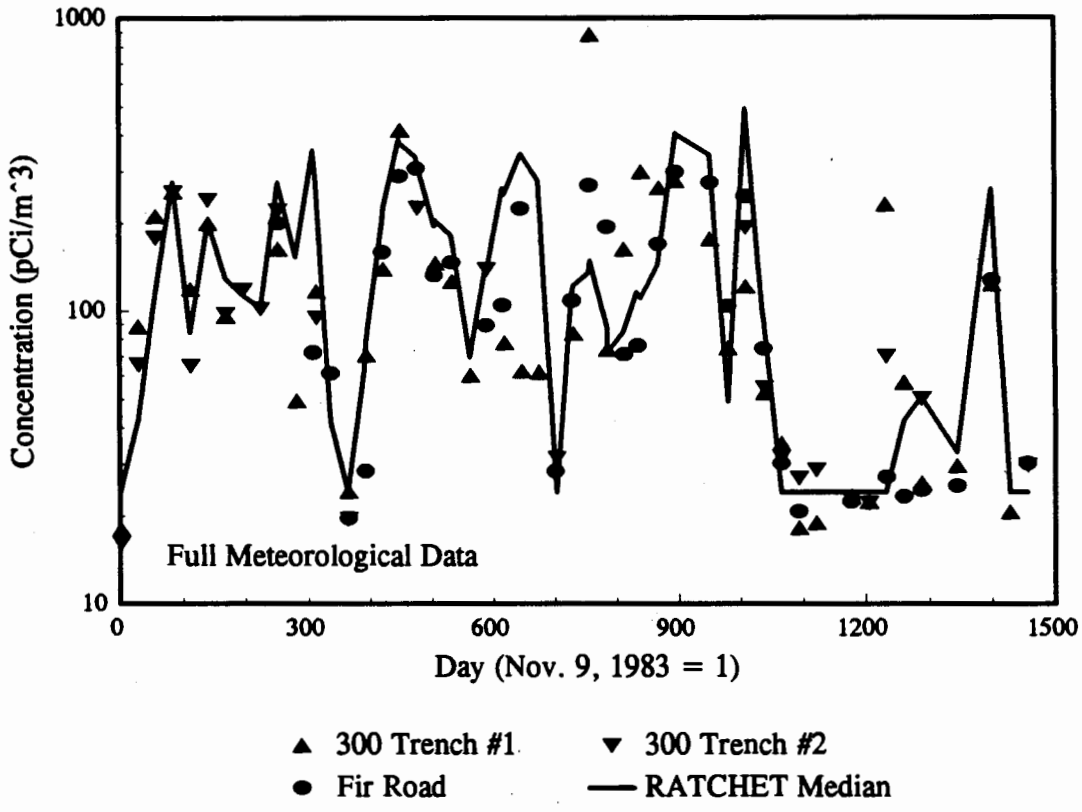

Figure 2.12. Comparison of the Measured Krypton-85 Concentrations at Node 17,23 with the Median Concentration Predicted by RATCHET, November 1983 - September 1987

300 Area Trench and Fir Road sampling locations. In general, the model results agree with the monitoring data. The median prediction gives concentrations of the correct order of magnitude and closely matches the temporal variations in the measured concentrations.

In Figure 2.13, the same concentration measurements are compared with the minimum and maximum concentrations predicted by RATCHET in the first set of 50 model runs (full meteorological data). The measured concentrations generally lie near, but are not necessarily within, the range of predictions.

Even ignoring the measured values near the background, there are more measured concentrations below the predicted range than above it. This indicates that the model is biased toward overprediction of concentrations. The fact that there are a relatively large number of underpredictions in spite of the apparent bias toward overprediction suggests that RATCHET tends to underestimate the range of uncertainty. However, RATCHET does not model the uncertainty associated with sampling. Sampling uncertainty suggested by the data shown in Figure 2.10 is a factor in RATCHET's apparent underestimate of the range of uncertainty in monthly average concentrations. Given this unmodeled source of variability, it is reasonable to conclude that the kryption-85 data indicate that RATCHET does not overestimate the uncertainty in monthly average concentrations but may underestimate it.

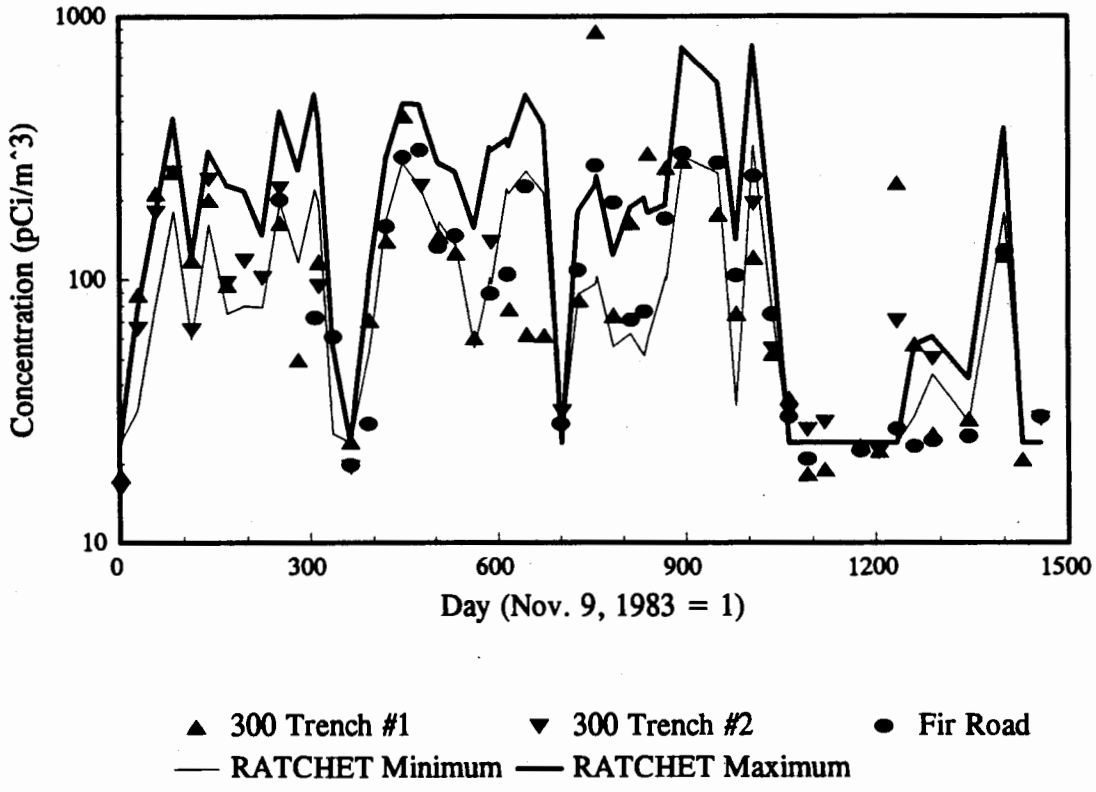

Figure 2.13. Comparison of the Measured Krypton-85 Concentrations at Node 17,23 with the Range of Concentrations Predicted by RATCHET, November 1983 - September 1987

2.9.6 Model Bias

The time series of concentrations for node 17,23 indicates that there is a bias in RATCHET's concentration estimates. Further information on potential model bias can be obtained by examining the bias at the individual monitoring locations for the entire period of record.

Table 2.5 shows the ratio of median predicted to measured time-integrated concentrations for each krypton-85 sampling location for both sets of RATCHET runs. When RATCHET was run with the full meteorological data set, the maximum ratio is 2.31 at the Ringold monitoring location. This ratio shows that on the average, the predicted concentrations are a factor of 2.31 too high. Biases at all of the other locations are less than a factor of two for the full meteorological data set. In no case is the ratio less than one, a situation that would indicate a bias toward underprediction. The overall model bias is a factor of 1.45 overprediction.

Table 2.5. Bias in RATCHET Median Estimates of Krypton-85 Concentrations

Monitoring Location	Monitoring Period	Number of Samples	Median Predicted/Measured Concentration	
			Full Met. Data	Limited Met. Data
300 Area Trench	1983-1987	42	1.12	2.06
	1983-1987	25	1.24	1.82
Fir Road	1984-1987	34	1.28	2.44
Prosser Barricade	1984-1987	28	1.62	1.43
Ringold	1983-1987	41	2.31	2.36
Sagehill	1984-1987	32	1.72	1.59
Pasco	1986-1987	22	1.16	1.23
Eltopia	1986-1987	15	1.62	3.31
Sunnyside	1984-1987	41	1.09	0.82
Yakima	1986-1987	18	1.13	0.89
	Overall	316	1.45	1.85

When RATCHET was run using limited meteorological data, the overall bias increases from 1.45 to 1.85. However, the increase in bias is not uniformly distributed among monitoring locations. The bias increases at six locations and decreases at five.

Figure 2.14 shows cumulative frequency distributions for the ratio between the median predicted concentration and the measured concentration for all samples and both sets of RATCHET runs. The distributions for the two sets of runs are similar. They show that the median ratio is about 1.25 when the full meteorological data set is used to predict concentrations and about 1.38 when the meteorological data are limited. In addition, median predicted concentrations are about 10 percent more

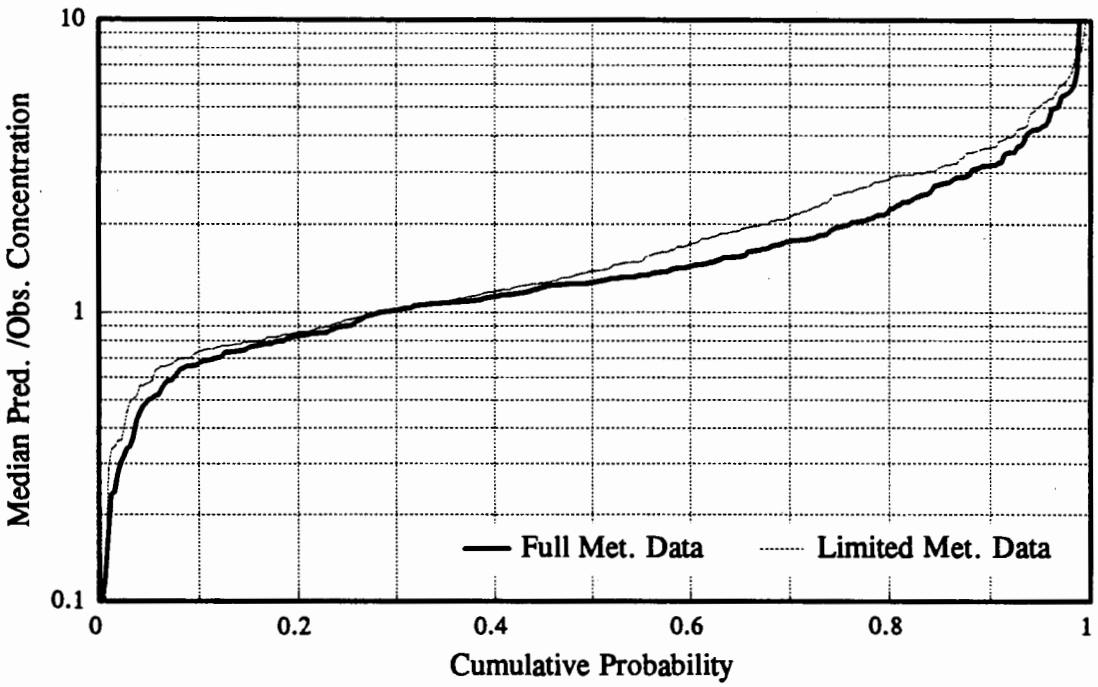

Figure 2.14. Cumulative Frequency Distributions for the Ratio between the Median Value of Predicted Concentrations and the Measured Concentrations in the Krypton-85 Data Set

likely to be within a factor of two of the measured concentration when the full meteorological data set is used (73 percent compared with 64 percent). However, running RATCHET with either meteorological data set resulted in more than 90 percent of the medians of the predicted concentrations being within a factor of four of the measured concentration.

2.10 Data Quality Objectives

Data quality objectives related to accuracy, precision, completeness, representativeness, and comparability have been established for the atmospheric transport model (Shipler 1993). The RATCHET code and input have been evaluated for completeness, representativeness, and comparability by numerous reviews. In an independent review conducted for the CDC,[(a)] the reviewers concluded

- that the modeling approach implemented in the RATCHET code was appropriate for the problem at hand

(a) Letter (HEDR Project Office Document No. 09930289), "Review of the Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)," from J.E. Till (TSP) to D. B. Shipler (BNW), July 12, 1993.

- that the appropriate atmospheric processes were included in the model
- that the representation of the science was consistent with present understanding and the constraints imposed by available meteorological data
- that they knew of no better code for use in the HEDR Project.

These findings indicate that RATCHET meets the data quality objectives for completeness, representativeness, and comparability.

Model accuracy and precision are evaluated in the HEDR model-validation studies (Napier et al. 1994). The final determination is based, in part, on comparisons of RATCHET concentration predictions with measured data in the krypton-85 data set, as discussed above. Seven additional data sets that do not include direct air concentration or deposition measurements (Napier 1994) provide indirect evidence related to model accuracy and precision.

The data quality objective for RATCHET related to accuracy is "...that bias in monthly time-integrated air concentrations and ground contaminations be less than a factor of three." The krypton data indicate that the bias in the median values of RATCHET predictions of air concentrations for nondepositing material is less than a factor of two. Furthermore, the data indicate that the median monthly-average concentration from a set of 50 model runs is within a factor of 3 of a measured concentration for more than 80 percent of the comparisons. These results suggest that RATCHET meets the data quality objective for accuracy of time-integrated air concentrations. RATCHET performance related to ground concentration will be evaluated as part of the evaluation of the environmental accumulation model, DESCARTES, and the dose calculation model, CIDER.

The data quality objective for RATCHET related to model precision is "...to characterize the uncertainty in time-integrated air concentrations and surface contamination resulting from uncertainty in the source term, meteorological data, and atmospheric model." The structure and components of the RATCHET code have been selected and implemented to meet this objective. Average air concentrations calculated by RATCHET vary over ranges of factors of two to five without accounting for the uncertainty in the source term. This variation in calculated concentrations is of the same magnitude as the variation among independent monthly average air samples collected at the same time at node 17,23. The results of preliminary studies of uncertainty suggest that uncertainty in the iodine source term will have an effect on the iodine air concentrations and deposition that is comparable to the uncertainty in the meteorological data and the model (Simpson and Ramsdell 1993).

3.0 RATCHET User's Guide

This chapter is a user's guide for Version 1.2 of the RATCHET computer code. All user interactions and data input are accomplished using data files. The sections in this chapter describe the input data files and their preparation, the output files, and program execution. The first section deals with the run-specification file; the second describes the selection of model parameters, the third section describes the remaining files used for data input. The fourth section describes the output files. The last two sections describe program control in a production environment and provide two sample problems.

3.1 Run-Specification File

The RUN SPECIFICATION FILE is the primary means of user input to the atmospheric transport code. The information in this file includes

- run identification
- model option controls
- input data file names
- output file names
- source characteristics and release rate file names
- effluent characterization
- random-number seeds.

The name of the file is stored internally in the character variable RS_FILE. A utility program, MAKE_RSF, creates run-specification files. Run-specification files may also be created or modified using an ASCII text editor.

The run-specification file contains 44 records when there is one source, and 3 more records for each additional source. Figure 3.1 shows the information in a typical run-specification file. The file in Figure 3.1 could be used to calculate the time-integrated air concentrations for the iodine-131 releases in January 1945. All records shown are mandatory, but the blank lines should not be included. They have been added to emphasize groups of related input. The record numbers, which are included in the figure for reference only, must not be included in an actual run-specification file. The comments following the slashes are included for reference. However, they are not part of the record. The precise format for each record is given in square brackets at the end of the comment in Figure 3.1 and again in parentheses as each record is discussed. All input begins in the first column. When several items are entered in one record, commas may be used to separate the fields.

Rec #	INPUT	COMMENT
1	HEADING..JAN 1945	/ Run identification [A80]
2	010145	/ Date to start model run segment [3I2]
3	0	/ Hour of the day to start run segment [I2]
4	013145	/ Date of end of segment [3I2]
5	24	/ Hour of end of segment [I2]
6	19312.128	/ Node spacing on envir. grid (m) [F10.0]
7	4	/ Number of puffs per hour [I2]
8	3	/ Min. time step index..see NSIA in DIFDEP [*]
9	T 1.5	/ Puff consolidation flag, criterion [L1,F10.0]
10	0	/ Computation option; 0 or 1 [*]
11	3.72	/ Maximum puff radius (σ_r units) [*]
12	1.0E-13	/ Minimum conc. at puff centers [*]
13	5.1, 10.3	/ Initial diffusion coefficients (m) [2F5.0]
14	0.5	/ σ_r coefficient for t > 60 min. [*]
15	N	/ Use constant mixing-layer depth [A1,F8.3]
16	44	/ Reference year for internal model clock [I4]
17	JAN45.MET	/ Meteorological data file [A40]
18	MSTA.DAT	/ Meteorological station file [A40]
19	MSTA_REV.DAT	/ Meteorological station revision of file [A40]
20	RP_DEC44.001	/ Puffs from previous run segment [A40]
21	HEDR_Z0.001	/ Surface roughness lengths [A40]
22	PRZONES.DAT	/ Precipitation zone definitions [A40]
23	PRATES.DAT	/ Precip.-rate frequency distributions [A40]
24	DEF_MIX.DAT	/ Default mixing-layer depth [A40]
25	STAB_DIS.DAT	/ Stab. class cum. freq. distributions [A40]
26	EX_JAN45.001	/ Primary output file name [A40]
27	NG_JAN45.001	/ Secondary output file name [A40]
28	RP_JAN45.001	/ Output residual-puff output file name [A40]
29	MBS.001	/ Monthly mass-balance summary file name [A40]
30	MPS.001	/ Monthly precipitation summary file name [A40]
31	1	/ Number of sources[I2]
32	-44.21, -6.89, 61.0	/ Position of source, release height [*]
33	0.792, 9.44, 25.0	/ Stack parameters, effluent temperature [*]
34	TQ.001	/ Release rate file [A40]
35	4	/ Effluent type [I5]
36	8.05	/ Half life (days) [*]
37	20.0, 30.0,50.0	/ Species partitioning in percent [3F10.0]
38	10000.0, 10.0, 100.0	/ Transfer resistances (sec/m) [3F10.0]
39	0.5, 1000.0	/ Solubility coefficients [2F10.0]
40	120983843.	/ Random-number seed for wind[*]
41	399287741.	/ Random-number seed for stab. class [*]
42	2873651.	/ Random-number seed for M-O length [*]
43	29084621.	/ Random-number seed for mix. depth [*]
44	98654321.	/ Random-number seen for precip rate [*]

Figure 3.1. Typical RATCHET Run-Specification File (January 1945)

3.1.1 Run-Segment Description

RATCHET is designed for climatological dispersion modeling. A single model run is expected to cover a period of several years. The code is structured to make long runs in short segments, rather than attempting to make them without interruption. The first group of records in the run-specification file defines the run segment.

The first record (A80) supplies a character string that is used to identify the model run. This string may contain as many as 80 characters. If the first character in the string is an asterisk, a program option will be activated that generates additional model output used for code verification. This output includes position, distance moved, diffusion coefficients, and mass in each puff at the end of each hour.

The second and third records specify the date and time, respectively, of the beginning of a model run segment. These values are used in searching the meteorological data file for the initial meteorological data record.

The date must be entered in the second record (3I2) as a six-digit integer in the form mmddyy, where mm is the month, dd is the day, and yy is the year. Leading zeros must be entered. The time must be later than January 1 of the reference year used for the model internal timing. The reference year is entered in the sixteenth record. If a time prior to January 1 of the reference year is entered, program execution will be aborted. Similarly, program execution will be aborted if either dd or mm is less than 1, if dd is greater than 31, or if mm is greater than 12.

The third record (I2) contains the hour that the run segment begins. For the purpose of this record, the day begins at hour 00 (midnight), and the last hour of the day is 23 (11 p.m.). Leading zeros may be dropped for the first 9 hours of the day. Entries less than 00 or greater than 23 will cause program execution to abort.

The fourth and fifth records contain the date and time of the end of the run segment. The date is contained in the fourth record (3I2) in the same form as the date for the start of the run segment. The fifth record (I2) contains the hour of the end of the run segment. This number is the last hour of the day to be completed and should be between 01 and 24.

3.1.2 Model Parameters

The second group of records in the run-specification file contains model parameters. These parameters set the size of the domain, set the puff release rate and diffusion computation time step, control consolidation of overlapping puffs, define puff dimensions, set a *de minimis* concentration in puffs, control calculation of the mixing-layer depth, and set the model reference time. This section briefly describes each of the records. Section 3.2 describes the sensitivity of RATCHET calculations to several of the parameters and provides guidance on selecting values for use in climatological studies.

The sixth record (F10.0) specifies the spacing between nodes on the environmental grid, which is stored in the variable DELXY. The spacing between nodes is entered in meters. It is the same in

both the x and y directions. The spacing between nodes on the concentration grid used for model output is one half the environmental grid spacing.

The seventh record (I2) specifies the number of puffs to be released each hour (NPH). The number entered must be an integer factor of 60. Tests on an early version of one of the predecessors to RATCHET (Ramsdell and Athey 1981) showed that three to six puffs per hour provide reasonable estimates of daily average concentrations. Fewer puffs can be used for climatological studies.

The eighth record (*) controls the minimum sampling interval (time step) used in diffusion and deposition computations. The maximum time step used in calculating puff movement is based on the puff release rate. It is 60/NPH minutes. However, puffs may be moved in smaller time steps to improve the accuracy of the summations used to approximate the time-integrated air concentrations and surface contamination. The number entered via this record is the index, IOPDTA, that controls the maximum number of time steps and, therefore, the minimum time step used to calculate concentrations. IOPDTA must be in the range from 1 through 12. The maximum number of sampling intervals which correspond to the index ranges are as follows:

INDEX	1	2	3	4	5	6	7	8	9	10	11	12
Max. Intervals	1	2	3	4	5	6	7	8	10	15	30	60

The minimum time step in minutes is 60 divided by the product of NPH and the maximum number of sampling intervals. The minimum time step is not necessarily an integer.

RATCHET's predecessors automatically consolidated overlapping puffs to reduce the code execution time. Puff consolidation is an option in RATCHET. Entries in the ninth record control the option. The first entry (L1) sets the value of the logical variable, CLN_FLG. If CLN_FLG is false, the puff consolidation option is disabled, and the second entry is ignored. If CLN_FLG is true, the second entry, CLN_CRIT sets the criterion used to determine when puffs are combined. Puffs from the same source are combined when the ratio of the separation between puff centers to the average σ_r is less than CLN_CRIT. RATCHET has two computational options. It computes time-integrated concentrations for a nondepositing, nondecaying gas in both options. This gas might be a long-lived noble gas such as krypton-85 or some other inert tracer. A1 should be entered in the tenth record (*) if this is the only computational product desired. The alternative is to enter a zero in the tenth record. Entering a zero in the tenth record enables computation of time-integrated air concentrations and surface contamination. In this case, the effluent may deposit and decay.

The Gaussian model will calculate extremely small concentrations at large distances from a puff center. These concentrations are insignificant compared to the concentrations near the center of the puff, but their calculation can significantly increase model execution time. The eleventh record (*) defines the maximum puff radius in terms of σ_r. Entering 3.72 in this record sets the maximum puff radius as $3.72\sigma_r$. With this definition, the concentration at the edge of the puff is 0.1 percent of the concentration at the center.

The twelfth record (*) in the run-specification file is a *de minimis* concentration. When the concentration at the center of a puff falls below this value, the puff is deactivated. This concentration should be sufficiently low to ensure that further exposure to the material in the puff could not contribute significantly to the dose received by any individual.

The thirteenth record (2F5.0) contains initial values for the diffusion coefficients. These values are most significant near the release point. They should be selected on the basis of the flow and concentration at the source so that initial concentration in puffs are approximately equal to the concentration at the source. Typical stack flows in the fuel-processing plants at the Hanford Site were 20,000 cfm. If σ_y is assumed to be equal to $2\sigma_z$ and NPH = 4, then 5.1 and 10.3 m are reasonable values for σ_z and σ_r, respectively. As a practical matter, with spacing between nodes on the environmental grid (DELXY) = 19,312 m, the initial values could be neglected for HEDR calculations without significantly affecting the monthly time-integrated air concentrations or surface contamination at nodes.

Record fourteen (*) in the run-specification file contains a constant (SY_CNST) used in the calculation of horizontal diffusion coefficients after the first hour. RATCHET computations are sensitive to the value of this parameter. Therefore, the parameter has been included in the run-specification file to permit its value to be changed without recompilation of the code. Section 3.2.6 deals with selection of values for this parameter.

The fifteenth record (A1,F8.3) controls the mixing-layer depth. If an N is entered via this record, the program will compute the mixing-layer depth used to limit vertical growth of the puffs from the meteorological data. Otherwise, if a Y is entered, the program will use a constant mixing-layer depth. This option is included to facilitate checking the operation of the code. The constant mixing-layer depth is entered following the Y.

The sixteenth record (I4) in the run-specification file, and the last record in the model parameter section, sets the reference time for the internal model clock. The internal model clock measures the elapsed time from midnight beginning the first of January of the year specified in the record. The year is specified by its last two digits.

3.1.3 Environmental Data Files

RATCHET uses nine files to define the physical environment within the model domain. The names of the nine files are entered in the seventeenth through twenty-fifth records of the run-specification file. These files are discussed in detail in Section 3.3. All file names are read with an A40 format.

The seventeenth and eighteenth records specify the names of files that contain the meteorological data and define the locations of the meteorological stations to be used in the model run segment. Both records must contain names of files that exist. If either file is missing or unreadable, program execution will abort. The nineteenth record is used to input the name of a file that contains updates to the meteorological station information. This file is optional, but the record must be included in the run-specification file even if it is blank.

The twentieth record is used to enter the name of a file that contains information on puffs that were active within the model domain at the end of the previous model-run segment. The information in this file is used to maintain continuity in a model run. The puff data file will not exist at the beginning of the first segment of a model run. Therefore, the file name should be left blank, but a blank record must be included in the run-specification file. If a file name is specified and the file is not found or cannot be opened, program execution will be aborted.

The twenty-first record in the run-specification file is used to enter the name of a file containing surface roughness lengths for each node on the environmental grid. The file is required. If the file named in this record does not exist, program execution will halt in an error mode.

The twenty-second and twenty-third records are used to enter names for files containing information related to precipitation regimes in the model domain. The file named in the twenty-second record is used to assign a precipitation regime to each node on the environmental grid. The twenty-third record contains the name of the file containing precipitation rate distributions for each of the precipitation regimes. Six distributions are required for each regime; one distribution for each of the precipitation types. This file also contains information to be used to adjust precipitation rates at nodes where the node is in a different precipitation regime than the meteorological station used to determine the precipitation type.

The twenty-fourth record is used to enter the name of a file containing default mixing-layer depths. The default mixing-layer depth file is required. If the file named in the record does not exist, program execution will halt in an error mode.

The last record in the environmental data file section of the run-specification file is used to enter the name of a file containing conditional cumulative probability distributions to be used in random sampling of stability classes. This file is required. If the file named in the record does not exist, program execution will halt in an error mode.

3.1.4 Output File Names

RATCHET creates six output files in the normal operational mode. In the testing mode, it creates one additional file. The name of the log file used to document code performance is automatically generated by RATCHET from the run-specification file name. RATCHET also generates the file name for test output when the code testing option is selected. RATCHET replaces the first two characters in the run-specification file name with "lg" to create the log file name and with "ts" to create the test file name. File names for the remaining five output files must be entered by the user in the twenty-sixth through thirtieth records of the run-specification file. All file names are read with an A40 format.

The name for the primary model output file is entered in the twenty-sixth record. This file will receive the daily time-integrated air concentrations and surface contamination to be used in subsequent calculations leading to dose estimates. The twenty-seventh record is used to enter the name of the file to receive the time-integrated air concentrations for nondecaying, nondepositing material. The twenty-eighth record is used to enter the name of the file to receive the information on puffs within the model domain at the end of the run segment. The name given to the twenty-eighth record at the

end of one run segment should appear as the file named in the twentieth record of the run-specification file for the next run segment.

The twenty-ninth and thirtieth records specify file names to receive information that may be used to evaluate model performance at a later date. The file named in the twenty-ninth record will receive information on the model mass balance at the end of each run segment. Information in this file includes estimates of the amount of material decaying in the air in transit, depositing within the model domain, and being carried out of the model domain. The file named in the thirtieth record receives the total precipitation estimated for each node during the run segment.

Use of a naming convention for the files specified in records 17 through 30 will facilitate file manipulation. The following convention is suggested. Data files, such as the meteorological station file, that will be the same for all production runs end in ".DAT." Meteorological data files, which are independent of realization but change monthly, are named MMMYY.MET where MMM is a three-letter abbreviation of the month, and YY is the last two digits of the year. Standard prefixes should be used to indicate file types for other files that change during the course of a model run. For example, EX may be used for the primary output files. Names for specific files are determined by adding an appropriate suffix to the file type. Files that change as a function of realization (e.g., the surface roughness file and the mass-balance summary file) have names that end in ".NNN" where NNN is the realization number. Finally, files that change as a function of both time and realization have names that end in "_MMMYY.NNN." For example, the file ex_dec44.001 would contain the RATCHET output to be used in dose calculation for the first realization of December 1944.

3.1.5 Source Characterization

The next group of records defines the source term or terms for the model. This group contains one record that gives the number of sources to be defined and three records for each source.

The thirty-first record (I2) in the run-specification file sets the number of sources to be considered by the model in the current run segment. From one to four sources may be specified. Each source requires three additional records. These three records define the source characteristics and provide the name of the file giving the release rates for that source.

The thirty-second record (*) contains the position of the source relative to the center of the environmental grid. It also contains the release height. Three entries are expected. The first two entries give the horizontal position of the release point relative to the center of the model domain. These positions are entered as distances east and north of the center in kilometers. Positions west and south of the domain center are entered as negative numbers. Release points must be within the model domain. The third entry is the height of the release point above the ground. It is entered in meters.

The thirty-third record (*) provides additional information about the source. It gives the stack radius in meters, stack flow in m^3/s, and effluent temperature in degrees Celsius. These three entries may be zero if the release is at ground level. However, the blank record must be included in the run-specification file.

The last record in this group (thirty-fourth record in the file) provides the name for a file that contains hourly release rate information for the source. The file name is read with an A40 format.

If more sources were specified, the last three records would be repeated for each source as a group. Definition of one source is completed before starting the definition of the next.

3.1.6 Effluent Characterization

RATCHET can simulate transport, diffusion, deposition, and decay of five types of effluents. The thirty-fifth through thirty-ninth records in the run-specification file define the effluent characteristics.

The thirty-fifth record (I5) defines the basic effluent type for the run segment. Table 3.1 defines general effluent type characteristics. The specific effluent characteristics, including half-life and dry and wet deposition, are controlled by data entered in the next four records.

Table 3.1. Effluent Type Characteristics

Type	Description	Deposit	Decay
0	Noble gas	No	Yes
1	Slightly reactive gas	Yes	Yes
2	Highly reactive gas	Yes	Yes
3	Small particles	Yes	Yes
4	Combined gas and particles	Yes	Yes

The thirty-sixth record (*) contains the half-life of the effluent. The half-life is entered in days. If the effluent does not undergo radioactive decay or if the half-life is long, a zero may be entered for the half-life.

The thirty-seventh record (3F10.0) is used to enter the fractions of type 4 effluents (combined gas and particles) that are associated with slightly reactive gases, reactive gases, and particles. The fractions are entered as percents in the order listed above. Table 3.2 summarizes information on partitioning of iodine in the atmosphere. For HEDR model runs, the fraction associated with particles is assumed to be uniformly distributed between 5 percent and 45 percent, and 20 percent to 60 percent of the gaseous iodine is assumed to be in reactive species. The remainder of the iodine is assumed to be in slightly or nonreactive gases. If the effluent is not type 4, the thirty-seventh record may be blank. However, the blank record must be included in the run-specification file.

The thirty-eighth record (3F10.0) is used to enter the transfer resistances used in the calculation of dry deposition velocities. These resistances place an upper limit on the deposition velocities. Guidance in selecting transfer resistances can be obtained from the review papers that summarize

Table 3.2. Partitioning of Iodine in the Atmosphere

Iodine Source (distance from source)	Iodine Associated with Particles (%)	Gaseous Iodine in Reactive Species (%)	References
Hanford Stacks	0 to 6	30 to 90	Perkins (1963) Ludwick (1967)
Hanford Expts (200-3200 m)	10 to 30	49 to 82	Ludwick (1964)
Hanford Plumes (5-8 km)	5 to 14	35 to 48	Ludwick (1964) Ludwick (1967)
Hanford Plumes (2-40 km)	4 to 42		Perkins (1963) Perkins (1964)
1949 Green Run (1-55 km)	6 to 39		Jenne and Healy (1950)
Chernobyl (> 1000 km)	7 to 54	11 to 54	Aoyama et al. (1986), Bondietti and Brantley (1986), Cambray et al. (1987), Mueck (1988), BIOMOVS (1990)
Natural Iodine	6 to 33	10 to 75	Voilleque (1979)

deposition measurements (McMahon and Denison 1979; Sehmel 1980). An approximate transfer resistance for a specific material can be estimated by finding the largest reported deposition velocity, converting it to meters per second, and taking the reciprocal of that value.

The thirty-ninth record (2F10.0) is used to enter solubility coefficients for type 1 and 2 effluents. These coefficients are related to the Henry's Law constants for the gases. Slinn (1984) discusses the calculation of solubility coefficients and lists values for several chemical species. Solubility coefficients of 0.5 and 1000 are used in the HEDR Project for the slightly reactive and highly reactive gases, respectively.

3.1.7 Random-Sampling Controls

The remaining group of records (*) in the run-specification file controls random sampling in the program. These records contain seeds for the pseudorandom-number generator. Random sampling is enabled by setting these seeds to values other than zero. The seeds should be large integers.

The first, second, and third seeds (fortieth, forty-first, and forty-second records) enable random sampling for wind directions and speeds, for stability classes, and for the reciprocal of the Monin-Obukhov length, respectively. Random sampling must be enabled for both stability classes and the reciprocal of the Monin-Obukhov length to get full representation of uncertainty related to

atmospheric stability. The fourth seed (forty-third record) enables random sampling for calculated mixing-layer depths. If a Y is entered in the fifteenth record, the use of variable mixing-layer depths is bypassed and entering a seed in this record will have no effect on model calculations. The fifth seed (forty-fourth record) enables random sampling for precipitation rates.

The use of random sampling for each variable is completely independent of the random sampling for the other variables. The random number seeds can all be 0, or one or more of the seeds may be nonzero. Selective use of nonzero seeds permits evaluation of model sensitivity to uncertainty in various model components.

3.2 Selection of Values for RATCHET Model Control Parameters

Selection of RATCHET parameters related to transport and diffusion is generally governed by available data. Other input is determined by the scenario under evaluation. This section discusses the selection of values for a group of parameters that are not defined by the available data or the scenario. Specifically, this section describes the sensitivity of the code execution time and time-integrated air concentrations and surface contamination to variations in several model parameters (e.g., NPH and IOPDTA) which were introduced in Section 3.1.2.

Model sensitivities to these parameters have been determined from calculations for the HEDR atmospheric transport model domain for the months of May 1945 and October through December 1949. Figure 2.1 shows the HEDR atmospheric transport model domain (DELXY = 19,312m) and the names of 50 locations within the domain. Monthly time-integrated air concentrations and deposition at these nodes are representative of the conditions throughout the model domain.

3.2.1 Number of Puffs per Hour

The seventh run-specification file record determines the number of puffs per hour (NPH) used in RATCHET to represent continuous plumes. The number of model calculations is directly related to the number of puffs released. However, Ramsdell and Athey (1981) indicate that increasing NPH beyond four to six does not result in a corresponding increase in precision of model calculations of daily concentrations. Figure 3.2 shows changes in time-integrated iodine-131 air concentrations and time required for code execution when NPH increases from 1 to 15. The time-integrated air concentrations at five locations are relatively insensitive to changes in NPH, while the time required for code execution increases almost linearly with NPH. Figures 3.3 and 3.4 compare time-integrated concentrations for all 50 locations computed with NPH = 3 and NPH = 4, respectively, with concentrations computed with NPH = 15. The solid diagonal lines in Figures 3.3 and 3.4 indicate perfect agreement between the model predictions. Also note that in some instances data points overlie each other. The results shown in Figures 3.2, 3.3, and 3.4 support use of NPH = 4 as an appropriate compromise between computational accuracy and code execution time.

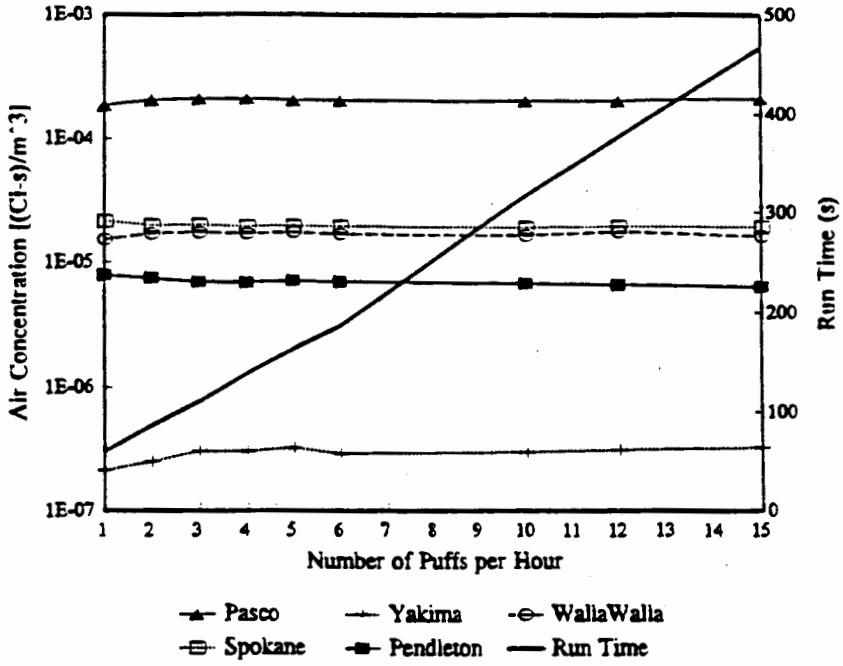

Figure 3.2. Variation of Time-Integrated Air Concentrations and Run Time as Functions of the Number of Puffs per Hour

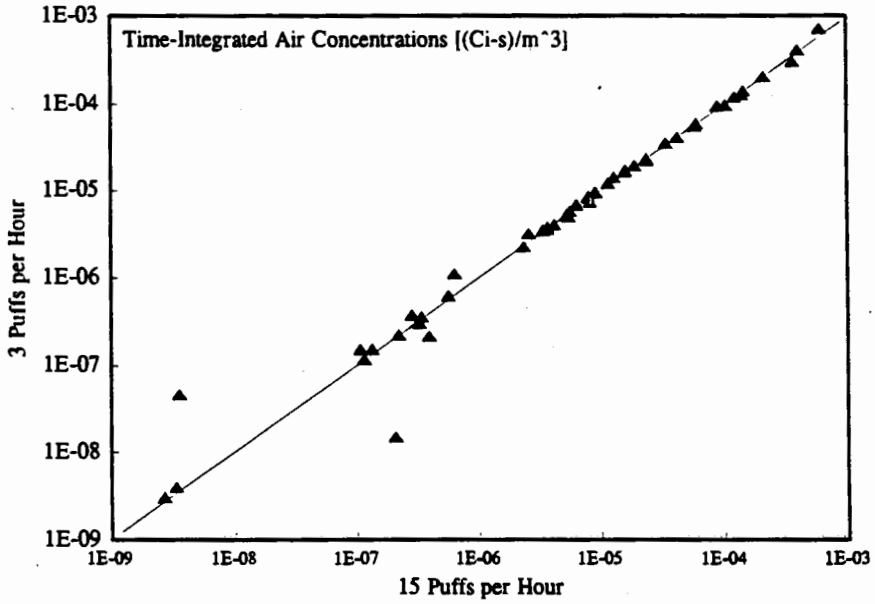

Figure 3.3 Comparison of Time-Integrated Concentrations for 50 Locations Computed with NPH=3 and NPH=15

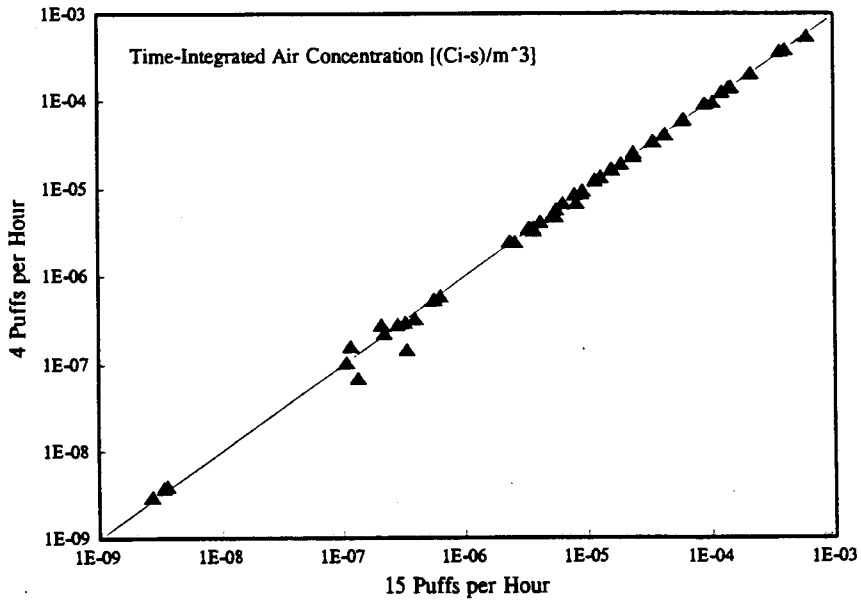

Figure 3.4. Comparison of Time-Integrated Concentrations for 50 Locations Computed with NPH=4 and NPH=15

3.2.2 Minimum Time Step for Calculations

Run-specification file record eight sets the minimum time step used in diffusion and transport calculations. The value entered via the record is an index (IOPDTA) that is used in determining the minimum time step given NPH and the puff σ_r. If IOPDTA is greater than one, the time steps used for young (small) puffs will be shorter than those used for old (large) puffs. Figure 3.5 shows the variation in May 1945 time-integrated air concentrations calculated for five nodes and code execution time as a function of the minimum time step. Changing the minimum time step does not have a significant effect on time-integrated air concentrations at these locations. Computational time does increase with decreasing minimum time step. However, the effect of IOPDTA on computational time is much less than the effect of NPH on computational time. Figure 3.6 compares time-integrated air concentrations computed for all 50 locations using 5-minute minimum time step with concentrations computed using 1-minute minimum time step. The solid diagonal line in Figure 3.6 indicates perfect agreement between the model predictions. The results in these figures suggest that use of a 5-minute minimum time step (NPH=4 and IOPDTA = 3) is reasonable.

3.2.3 Puff Consolidation

The RATCHET code includes an option to combine puffs that cover essentially the same area to decrease code execution time. This option is elected by setting the puff consolidation flag in record 9 to true and entering a minimum separation criterion, CLN_CRIT in the same record. The parameter CLN_CRIT is the ratio of the separation between puffs divided by the average σ_r of the puffs that separates the conditions when puff consolidation occurs and when it does not occur. The puff consolidation criterion is applied to puffs from the same source. When the ratio of the separation

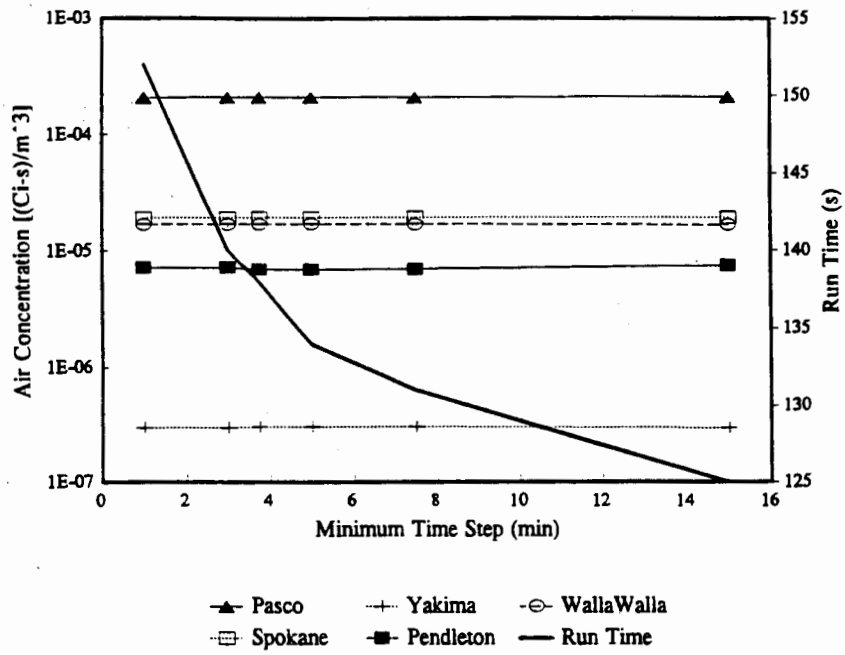

Figure 3.5. Variations in Time-Integrated Air Concentrations and Code Execution Time as Functions of the Minimum Time Step

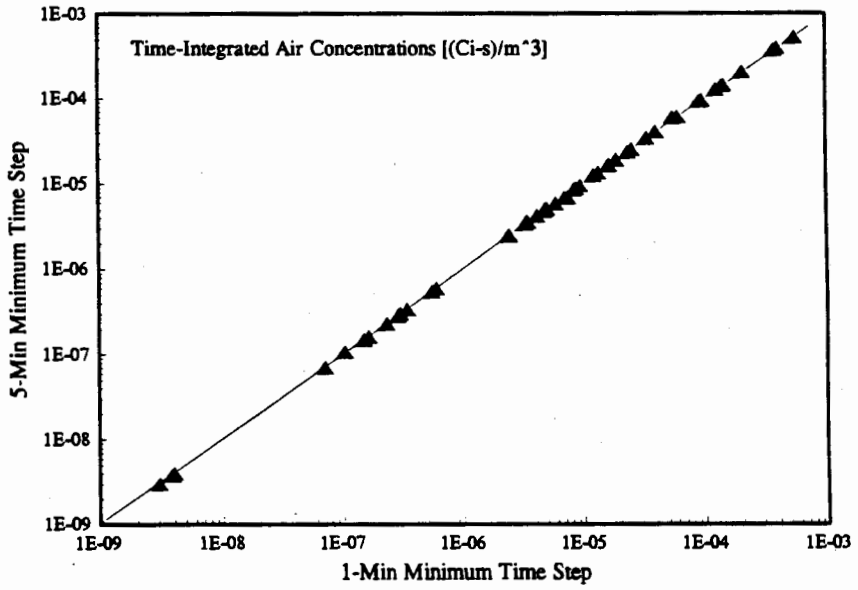

Figure 3.6. Comparison of Time-Integrated Concentrations for 50 Locations Computed with 1-Minute and 5-Minute Minimum Time Steps

between puffs to the average σ_r is less than CLN_CRIT, the puffs will be combined, and the consolidated puff will be placed at the center of mass of the original puffs.

As intended, puff consolidation significantly reduces code execution time. For example, without puff consolidation, the time required to simulate May 1945 averages about 5400 seconds. With consolidation of puffs and CLN_CRIT equal to two, the time is reduced to about 130 seconds. However, puff consolidation does have an effect on concentrations at specific locations. Figure 3.7 shows Realization 003 of May 1945 calculated with various CLN_CRIT values. It shows the effect on total surface contamination and run time of increasing CLN_CRIT from zero (no consolidation) to two. Increasing CLN_CRIT reduces the run time by a factor of more than 40, but only changes the surface contamination at these nodes by a few percent.

Figures 3.8 and 3.9 provide a more complete picture of the effect of puff consolidation on surface contamination for May 1945. These figures show the average and standard deviation, respectively, of the estimates of surface contamination for five realizations of May 1945 with and without consolidation. The consolidation criterion for these calculations was 1.5.

Figure 3.8 provides a strong indication that puff consolidation does not have either a large or systematic effect on the average surface contamination determined from a number of realizations in the main portion of the monthly plume footprint. The only nodes for which the differences might be significant are on the edges of the footprint, and they have little contamination in any of the realizations. The differences in standard deviations with and without consolidation shown in Figure 3.9

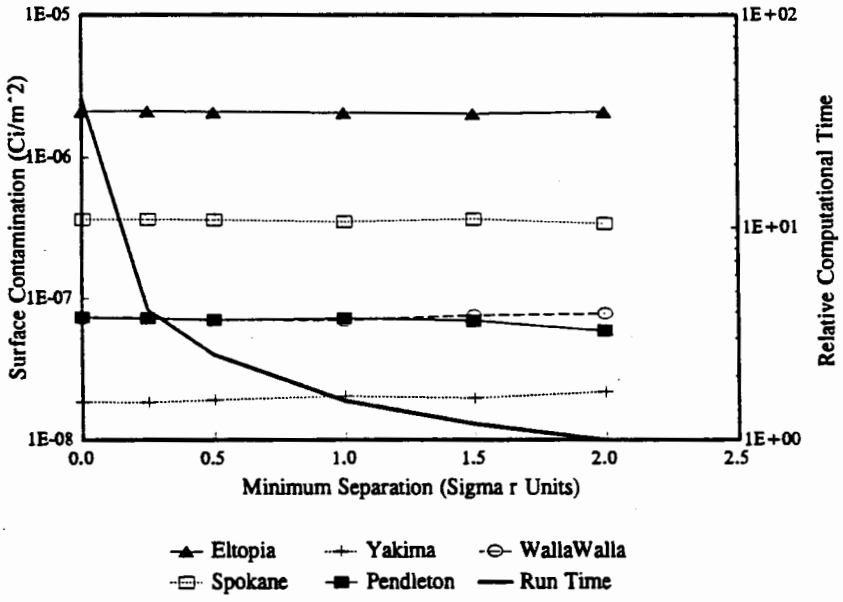

Figure 3.7. Variation of Surface Contamination and Code Execution Time as Functions of the Minimum Separation between Puffs

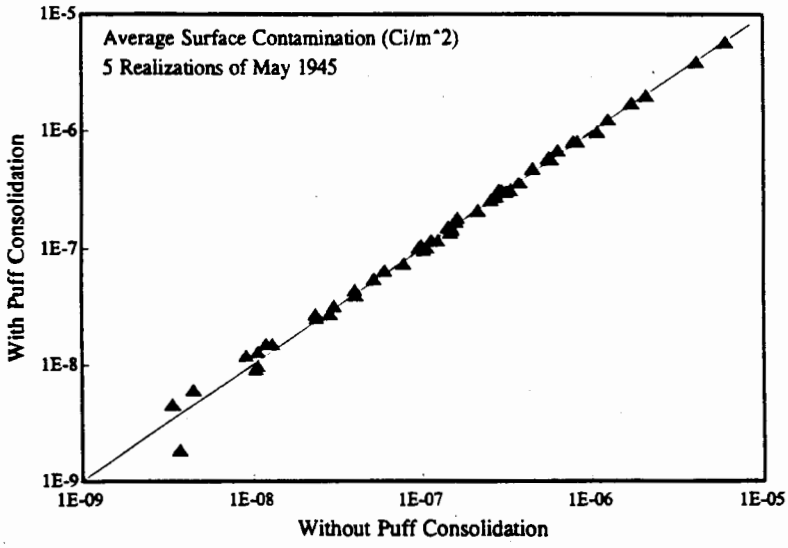

Figure 3.8. Effect of Puff Consolidation on the Average Surface Contamination at 50 Locations Based on Five Realizations

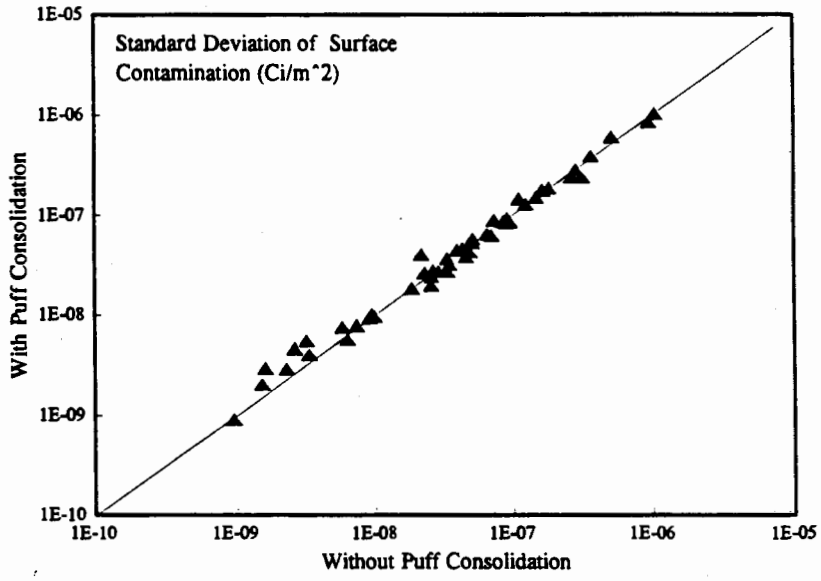

Figure 3.9. Effect of Puff Consolidation on the Standard Deviation in Surface Contamination at 50 Locations Based on Five Realizations

are larger than the differences in the averages. However, this increase may be due to the small number of realizations used in the comparison rather than to real differences in the spread of the distributions of the surface contamination at the nodes. At nodes with high contamination, consolidation does not appear to change the standard deviations systematically. The apparent increase in standard deviation with consolidation at nodes with low contamination may be real, or it may be an artifact of the small number of realizations. If the increase is real, it is not likely to be a significant factor in calculation of doses. Thus, the conclusion to be drawn from Figures 3.7 through 3.9 is puff consolidation within the limits tested significantly reduces RATCHET execution time without having a large or systematic impact on the precision of the calculations.

3.2.4 Puff Radius

The Gaussian curve has infinite tails. Therefore, when Gaussian models are used for dispersion calculations, the distribution has to be truncated at some point to avoid calculating a large number of extremely low concentrations. These concentrations are generally meaningless, while their calculation is time consuming.

May 1945 data have been used to determine the sensitivity of monthly time-integrated values and computational time to choice of the truncation point. During initial development, the concentrations were calculated for nodes within 5.3 σ_r of the center of each puff. Concentrations at distances greater than 5.3 σ_r were assumed to be zero. With this assumption, the ratio of the minimum concentration in a puff to the concentration at the puff center was $1x10^{-6}$. Figure 3.10 shows the effect of decreasing the maximum puff radius. Monthly surface contamination is very insensitive to the puff

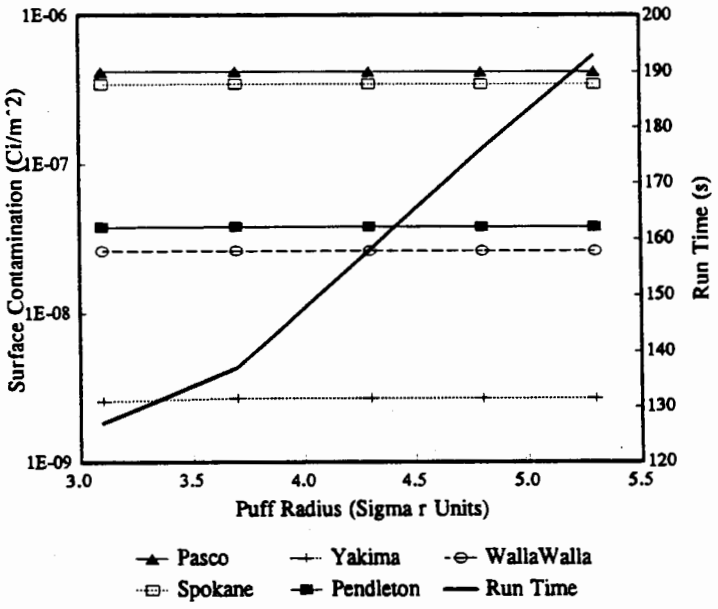

Figure 3.10. Effect of Decreasing Maximum Puff Radius on Calculating Surface Contamination and on Run Time

radius within the range evaluated, while the computational time is directly related to puff radius. Decreasing the puff radius from 5.3 σ_r to 3.7 σ_r results in a 30-percent reduction in run time.

Further decreases in puff radius do not yield comparable reductions in run time because the time required for preparation of the meteorological fields sets a lower bound on the run time. Figure 3.11 compares surface contamination at all 50 named nodes for puff radii of 3.7 σ_r and 5.3 σ_r.

Figures 3.10 and 3.11 clearly demonstrate that the changes in surface contamination that result from changes in puff radius are small compared to the range of values within the model domain. Thus, using a puff radius of 3.7 σ_r instead of 5.3 σ_r will not have a significant impact on the precision of model calculations. Truncating puffs at 3.7σ_r gives a concentration at the puff edge that is three orders of magnitude lower than the concentration at the center.

3.2.5 De Minimis Concentration

RATCHET uses a *de minimis* concentration as another means of limiting the number of calculations and thereby decreasing the run time. Nominal dose conversion factors may be used in selecting a *de minimis* concentration. For example, using the breathing rates and inhalation dose conversion factors for iodine-131 in Snyder et al. (1992), the inhalation dose to the thyroid is on the order of 200 to 300 rad per Ci-s/m^3 of exposure. Ingestion doses from locally-produced milk may be two orders of magnitude larger than the inhalation dose. Thus, if you assume that annual thyroid doses are the primary concern and that doses of less that one mrad are negligible, a simple calculation indicates that the concentration of iodine-131 in a puff must exceed about 1E-13 (1 x 10^{-13} Ci/m^3) before iodine-131 doses would be of concern, even with continuous exposure. The HEDR Technical Steering Panel has set an annual thyroid dose cut-off level at 1 rad.

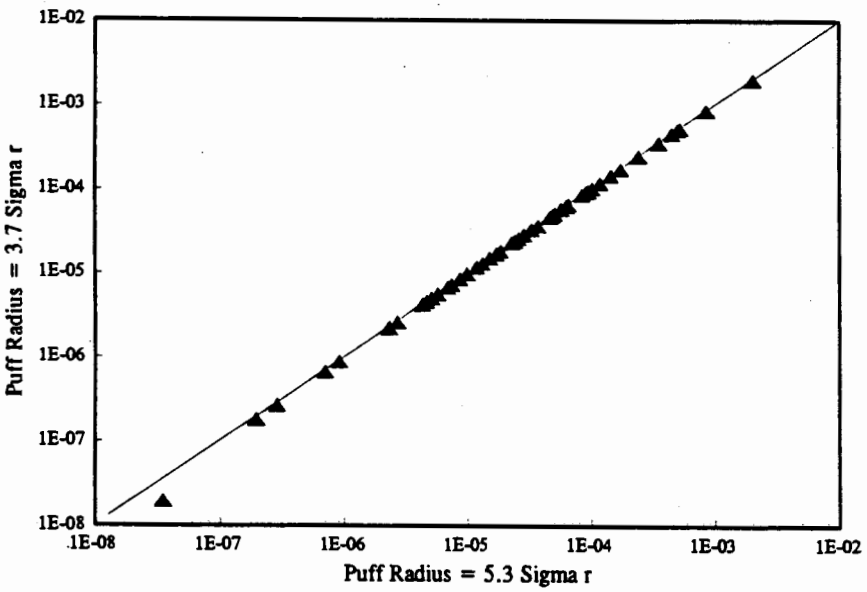

Figure 3.11. Comparison of Calculated Surface Contamination Values for Puff Radius = 3.7 σ_r and Puff Radius = 5.3 σ_r

3.2.6 Horizontal Diffusion Coefficient Proportionality Constant

In RATCHET, the horizontal diffusion coefficient is assumed to be proportional to time. For the first hour after a puff is released, the proportionality constant is a function of atmospheric turbulence and those parameters that affect the turbulence. After the first hour, factors other than atmospheric turbulence (e.g., wind shear) control horizontal diffusion. These factors are not modeled explicitly in RATCHET. However, their effect on horizontal diffusion is modeled implicitly in the proportionality constant used in calculating increases in the diffusion coefficient after the first hour. This dimensional constant, SY_CNST, is entered via record 14 of the run-specification file. In the HEDR Project, SY_CNST is assumed to be a random variable and is changed as a function of realization. Long-range diffusion data summarized by Gifford (1983) suggest the distribution in Table 3.3 with a median value of about 0.5 meters per second. This section discusses sensitivity of model calculations and run time to the value of SY_CNST.

Table 3.3. Distribution for Horizontal Diffusion Coefficient, SY_CNST

SY_CNST Range (m/s)	Probability (%)
0.14 to 0.28	20
0.28 to 0.56	60
0.56 to 1.40	20

Large values of SY_CNST are associated with large puffs and low concentrations at the puff center, while small values of SY_CNST are associated with small puffs and high concentrations at puff centers. Thus, changing SY_CNST has two effects on time-integrated air concentrations and deposition at nodes. It changes the frequency of exposure at nodes, and it changes the concentrations during the exposure period.

Model studies indicate that time-integrated air concentrations and surface contamination on the edges of the monthly exposure patterns are more sensitive to the value of SY_CNST than the values in the centers of the patterns. Figure 3.12 shows the effect on time-integrated concentration estimates at five nodes for December 1949 of changing SY_CNST. At the four nodes located near the centerline of the pattern (Pasco, Walla Walla, Spokane, and Pendleton), the total deposition tends to decrease as SY_CNST increases. At the fifth node, Yakima, which is located on the western edge of the pattern, the deposition increases by more than two orders of magnitude with about a factor of five increase in SY_CNST. This increase is the result of a general broadening of the pattern. Large values of SY_CNST tend to reduce gradients of time-integrated air concentrations and deposition. This effect is seen in Figure 3.12 in the decrease in difference in deposition between Pasco and Yakima as SY_CNST increases.

The effect of SY_CNST on run time in the normal RATCHET operational mode with puff consolidation is also shown in Figure 3.12. Increasing SY_CNST from about 0.15 to 1.1 increases the run time by about 60 percent. This increase is caused by the increase in area covered by each

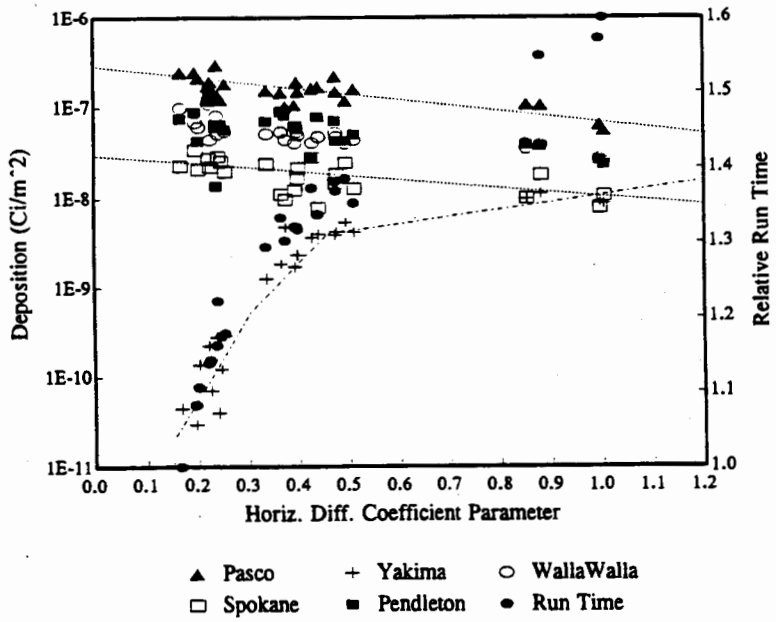

Figure 3.12. Effect of Changing SY_CNST on Deposition and Code Execution Time

puff. When RATCHET is run without puff consolidation, the range of run times increases to more than a factor of three. Figure 3.13 compares the relationship between run time and SY_CNST with and without puff consolidation.

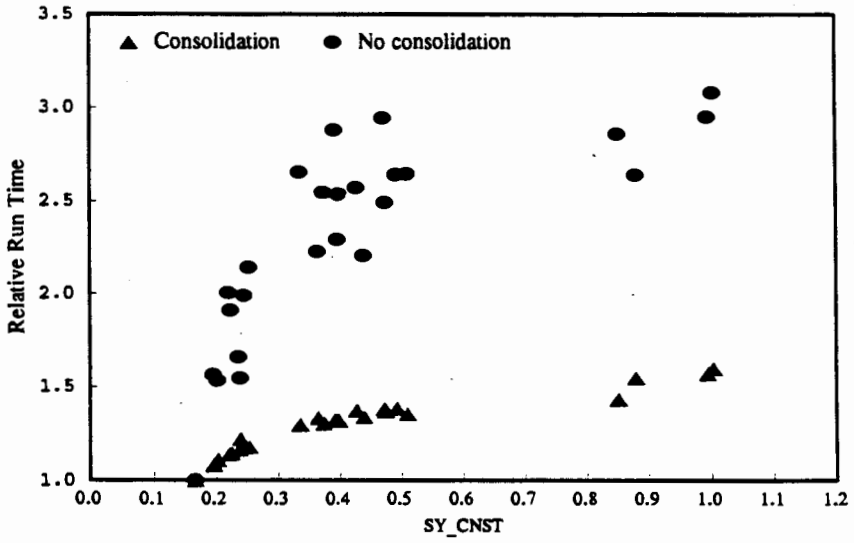

Figure 3.13. Relationship Between Run Time and SY_CNST With and Without Puff Consolidation

3.3 Input Files

Eleven input files are used in RATCHET. The files and file characteristics are listed in Table 3.4. The first section of the user's guide discussed the run-specification files used to control the model execution. This section discusses the ten remaining files.

Table 3.4. Summary of RATCHET Input Files

File Name	Access	Form	Status
Run Specification	Sequential	Formatted	Required
Surface Roughness Lengths	Sequential	Unformatted	Required
Precipitation Regime Definition	Sequential	Formatted	Required
Precipitation Rate Distribution	Sequential	Formatted	Required
Default Mixing Layer	Sequential	Formatted	Required
Stability Class Distribution	Sequential	Formatted	Required
Meteorological Stations	Sequential	Formatted	Required
Meteorological Station Revision	Direct	Formatted	Optional
Meteorological Data	Direct	Formatted	Required
Source-Term Data	Direct	Formatted	Required
Residual-Puff Data	Sequential	Unformatted	Optional

Three types of files are used for data input. These are formatted, sequential files; formatted, direct access files; and unformatted, sequential files.

Formatted, sequential files are used for data entered once per model run. They can be prepared using a text editor or a computer program. They can be displayed on terminals, and they can be printed directly.

Formatted, direct access files are used for data that are entered periodically during the code execution. Direct access files must be generated using a computer program. However, they may be displayed and printed. When direct access files are displayed or printed, one line is used for each record. As a result, the ends of the records may not be seen.

Unformatted, sequential files are used to pass data between components of the overall HEDR project model, with one exception—the surface roughness length file. The order, type, and dimension of variables in the statements writing and reading the files must be read identically to be successful. In general, unformatted files are difficult to interpret unless they are converted by a program.

3.3.1 Surface Roughness Length File

The surface roughness length is a characteristic length that enters into many atmospheric boundary layer calculations. It arises as a constant of integration in the derivation of the logarithmic wind profile. Section 2.2.1 describes the surface roughness length in more detail, and Table 2.1 relates surface roughness lengths to topographic and land use characteristics.

The surface roughness length file contains two records. The first record is a file heading, and the second record is an array of roughness lengths. The heading is a 60-character string and should contain information to uniquely identify the file contents. The surface roughness length array contains one element for each node on the environmental grid. The order of elements in the file is important. The first element must be the roughness length for the node in the southwest corner of the grid. The next element must contain the roughness length for the node immediately to the east of the first. This pattern continues until the roughness length for the southeast corner node is entered. After the surface roughness length for the southeast corner node is entered, the roughness length is entered for the node immediately north of the southwest corner node. This pattern is continued until the surface roughness is entered for the last node. The last node should be the node in the northeast corner of the grid.

The surface roughness length file is an unformatted file. A listing of a simple utility program for creating the file is available with the program listings.

3.3.2 Precipitation Regime Definition File

Precipitation can contribute significantly to deposition of radionuclides and thereby increase ingestion doses. RATCHET includes wet deposition algorithms that require estimates of precipitation rates. Initially RATCHET assumed that a single set of conditional distributions could be used to describe precipitation rates given the reported weather type. This approach underestimated precipitation in many locations. As a result, the precipitation model was expanded to include three precipitation regimes and a different set of precipitation rate distributions for each regime.

For the HEDR Project, the precipitation regimes have been defined using the annual precipitation patterns defined in climatological documents, such as Climates of the States (Water Information Center 1974). Precipitation regime 1 is that region of the model domain having 10 inches of precipitation or less per year. Precipitation regime 2 includes the area with annual precipitation between 10 and 20 inches per year, and regime 3 is the area with more than 20 inches of precipitation per year.

Precipitation regime definitions are entered for each node of the environmental grid via the file named in record 22 of the run-specification file. The initial record in the file contains a heading (A60) that may be used to identify the file contents, date of preparation, source of data, etc. This heading is written to the log file. The remaining records contain integers that represent the precipitation regime at the environmental grid nodes. The precipitation regimes are read from west to east starting at the northernmost row of nodes using a 3X,21I2 format. Figure 3.14 shows a precipitation regime file. The integers in the left column are included to facilitate identification of specific nodes.

```
Precipitation Zones based on Annual Average Precip Amounts
26  3 3 3 3 3 3 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3
25  3 3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3
24  3 3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3
23  3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3
22  3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3
21  3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3
20  3 3 3 3 2 2 2 1 1 1 1 2 2 2 2 2 2 2 2 3 3 3
19  3 3 3 2 2 1 1 1 1 1 1 1 2 2 2 2 2 2 2 3 3 3
18  3 3 2 2 1 1 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3
17  3 3 2 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3
16  3 3 2 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 3 3 3 3
15  3 3 2 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 3 3 3 3
14  3 3 2 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 3 3 3 3
13  3 3 2 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 3 3 3 3
12  3 3 2 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3
11  3 3 2 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 3 3
10  3 3 2 2 2 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2
9   3 2 2 2 2 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2
8   2 2 2 2 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2
7   2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
6   2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3
5   2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3
4   2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3
3   2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3
2   1 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3
1   2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3

    1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1
```

Figure 3.14. Sample Precipitation Regime Data File

They are skipped by the formatted read statement in RATCHET. The bottom row of integers is included in the file for the same reason. It is not read by the program.

3.3.3 Precipitation Rate Distribution File

Conditional precipitation rate distributions are required for each precipitation type and precipitation regime. The conditional distributions provide a method of translating the current weather observation in standard meteorological reports to precipitation rates. They can be generated from climatological data. Conditional precipitation distributions for the HEDR Project were developed in two ways. The first was direct estimation of the distributions from records of hourly weather observations at HMS. These records contain both current weather observations and hourly precipitation amounts. The second way of developing the distributions was to use the hourly weather observations to determine current weather and to obtain the corresponding precipitation amounts from

monthly summaries of local climatological data. Hourly data and the corresponding monthly summaries were available for Yakima, Pendleton, Spokane (Felts Field), Lewiston, and Stampede Pass. Data from HMS and Yakima were combined to estimate the conditional frequency distribution for precipitation regime 1. Data from Pendleton, Spokane, and Lewiston were used for regime 2, and data from Stampede Pass were used for regime 3.

The cumulative frequency distributions are entered via the file named in the twenty-third record of the run-specification file. The first record in the file (A60) is a header record. It may be used to identify the file contents, date of preparation, etc. The next 18 records contain information on the distributions. These records are read using a 5X,12F5.0 format. The final record is used for entering adjustment factors to compensate for differences in precipitation regimes between nodes and the closest meteorological station. It is also read using a 5X,12F5.0 format.

Figure 3.15 shows a sample precipitation rate distribution file. The first 2 columns shown in records containing the distribution information are the precipitation type and precipitation regime, respectively. These columns are included in the file for clarity, but skipped when the file is read. The remaining 12 columns alternate between precipitation rate and cumulative frequency. All precipitation rates are in inches per hour, water equivalent. The frequencies are upper limits for precipitation rate bands.

```
Precipitation Rate Data for HEDR Precipitation Zones 1-3
1  1     .01   .581  .02   .433  .04   .781  .07   .939  .10   .974  .15  1.00
2  1     .01   .000  .09   .063  .14   .594  .18   .750  .30  1.00   .45  1.00
3  1     .01   .000  .09   .063  .14   .594  .18   .750  .30  1.00   .45  1.00
4  1     .01   .690  .02   .444  .04   .820  .07   .956  .10   .994  .15  1.00
5  1     .01   .000  .03   .043  .06   .478  .10   .913  .14  1.00   .15  1.00
6  1     .01   .000  .03   .043  .06   .478  .10   .913  .14  1.00   .15  1.00
1  2     .01   .483  .02   .357  .04   .697  .07   .885  .10   .957  .15  1.00
2  2     .01   .000  .08   .081  .14   .581  .20   .823  .25   .903  .45  1.00
3  2     .01   .000  .08   .081  .14   .581  .20   .823  .25   .903  .45  1.00
4  2     .01   .650  .02   .473  .04   .819  .07   .975  .10   .994  .15  1.00
5  2     .01   .000  .07   .733  .10   .933  .12  1.00   .15  1.00   .15  1.00
6  2     .01   .000  .07   .733  .10   .933  .12  1.00   .15  1.00   .15  1.00
1  3     .01   .345  .02   .295  .04   .598  .07   .878  .10   .959  .15  1.00
2  3     .01   .000  .11   .044  .14   .415  .17   .648  .23   .906  .32  1.00
3  3     .01   .000  .10   .000  .31   .158  .32   .526  .46  1.00   .50  1.00
4  3     .01   .308  .02   .303  .04   .739  .07   .870  .10   .967  .15  1.00
5  3     .01   .000  .04   .000  .08   .067  .11   .176  .16   .728  .28  1.00
6  3     .01   .000  .04   .000  .08   .067  .11   .176  .16   .728  .28  1.00
   1.00  2.00  4.00  0.50  1.00  2.00  0.25  0.50  1.00
```

Figure 3.15. Sample Precipitation Rate Distribution File

The first pair of entries for precipitation type 1 (light rain) in precipitation regime 1 is 0.01, 0.581. The first precipitation rate band deals with accumulations of less than 0.01 inch in an hour. This band accounts for all of the hours with trace amounts of precipitation. The 0.581 indicates that 58.1 percent of the hours with light rain resulted in a total accumulation of a trace. The first pair of entries in each of these records deals with trace precipitation amounts. The remaining fields in the records deal with precipitation rates greater than a trace. The cumulative frequencies in these fields are based on hourly data with accumulations of 0.01 inch of precipitation or more. Thus, 43.3 percent of the time when there is light rain in precipitation regime 1, the hourly accumulation is less than 0.02 inches. Similarly, the probability that hourly accumulation is less than 0.04 inches is 78.1 percent.

The last pair of fields in each record containing the precipitation rate distribution rate information defines an upper limit for the precipitation type and regime. This is accomplished by setting the maximum rate in the next to the last column and setting the cumulative probability in the last column equal to 1.00. If the precipitation rate distributions can be defined adequately with less than five bands, the upper limit may be set at any time. In the example file above, an upper limit of 0.30 inches per hour is set for moderate rain (precipitation type 2) in precipitation regime 1. The example file also shows several instances where the same distribution is used for more than one precipitation type. In these cases there is insufficient information on which to base a separate distribution for the types with heavier precipitation.

The final record contains adjustment factors used to modify precipitation rates to account for differences in precipitation regimes between a node and the closest meteorological station. Selection of these factors is subjective, although the conditional frequency distributions may provide some insight into the selection process. These factors are read into a three by three array. The first index of the array corresponds to the precipitation regime at the node, and the second index corresponds to the precipitation regime at the meteorological station. If the indexes are the same, the adjustment factor should be 1. If the node index is greater than the meteorological station index, the adjustment factor should be greater than 1, and if the node index is less than the station index, the adjustment factor should be less than 1.

3.3.4 Default Mixing-Layer Depth File

The default mixing-layer depth file is a formatted, sequential file that contains 60 records. Each record contains the default mixing-layer depths for one stability group and month. Eight fields within the record give the variation in default mixing-layer depth with the time of day. The format for the records is 11X, 8F7.1. The default mixing-layer depth file may be created with a text editor.

Only five stability classes are used for determining the default mixing-layer depth. For the purposes of determining the default mixing depth, stability class combines the two extremely unstable classes (1 and 2) used in the remainder of the program. Stability classes 2, 3, and 4 correspond to original stability classes used in the remainder of the program minus 1. The remaining stability class (5) includes the original stability classes 6 and 7.

Figure 3.16 shows the first 15 records of a default mixing-layer depth file based on mixing-layer depth estimates made by HMS forecasting staff from 1983 through 1987. The first set of five records

0.	0.	0.	225.	225.	0.	0.	0.
0.	0.	175.	300.	300.	0.	0.	0.
900.	900.	750.	750.	750.	750.	750.	750.
275.	300.	300.	0.	0.	350.	275.	225.
200.	175.	150.	0.	0.	200.	150.	175.
0.	0.	175.	275.	375.	0.	0.	0.
0.	0.	175.	375.	475.	275.	0.	0.
700.	700.	700.	800.	1000.	750.	750.	700.
225.	225.	225.	0.	0.	375.	225.	225.
150.	175.	150.	0.	0.	225.	175.	150.
0.	0.	200.	450.	600.	500.	0.	0.
0.	0.	250.	525.	725.	550.	0.	0.
550.	550.	550.	1025.	1125.	850.	625.	625.
300.	250.	225.	0.	0.	550.	300.	300.
175.	175.	150.	0.	0.	325.	175.	175.

Figure 3.16. Default Mixing-Layer Depths at the Hanford Site for January through March

is for January, the next set of five is for February, etc. Within each set of five records, the first record is for the most unstable atmospheric conditions. Each succeeding record represents an increase in stability. The time of day is represented by the columns, starting with midnight to 3:00 a.m. in the first column.

3.3.5 Stability Class Cumulative Frequency Distribution File

The stability class cumulative frequency distribution file is a formatted, sequential file that contains seven records. Each record contains the cumulative frequency distribution for the possible actual stability class for one reported stability class. The format for the records in the file is 1X, 7F7.4.

Figure 3.17 shows a stability class cumulative frequency distribution file based on five years of data at HMS. The first record contains the cumulative frequency distribution for actual stability classes given a reported stability class of 1; the third record has the distribution given a reported

0.8950	0.9286	0.9454	1.0000	1.0000	1.0000	1.0000
0.5971	0.7174	0.7862	0.9634	0.9864	0.9972	1.0000
0.3776	0.4922	0.5785	0.8358	0.9133	0.9682	1.0000
0.1316	0.1716	0.2158	0.6059	0.8695	0.9654	1.0000
0.0007	0.0015	0.0032	0.1080	0.4726	0.8335	1.0000
0.0005	0.0019	0.0033	0.0805	0.4027	0.7931	1.0000
0.0000	0.0009	0.0017	0.0706	0.3540	0.7724	1.0000

Figure 3.17. Stability Class Cumulative Frequency Distribution File Based on Comparison of Classes Estimated from Climatology with Classes Estimated by Temperature Lapse Rate at HMS 1983-1987

stability class of 3, etc. When random sampling of stability classes is selected in the run-specification file, the input stability class for a station is used as the row index and the column index is set to 1. The random number generated by RATCHET is compared with the value at this location in the array. If the random number is greater than the value at the location, the column index is increased by 1 and the comparison is repeated. This process continues until the value in the array exceeds the random number. When this occurs, the column index becomes the output stability class. The stability class cumulative frequency distribution file may be created with a text editor.

3.3.6 Meteorological Station File

Meteorological station locations are entered via the meteorological station file specified in the eighteenth record of the run-specification file. This file is a formatted, sequential access file that may be created and edited with a text editor. A simple utility program has been created to prepare meteorological station files. The program is called MAKE_STA and is included with the program listing. Meteorological station files can also be created with a text editor. The meteorological station file must include an entry for each location for which meteorological data are available. The order of the station locations must correspond to the order of the data in the meteorological data file.

Records in the file contain the station name, the position of the station relative to the center of the domain, and the height of the wind measurement. They also contain an estimate of the surface roughness at the station, wind reporting unit indicators for direction and speed, and a status flag. The format for the file is 1X, A4, 2F10.0, 2F7.0, 1X, 3I4.

Station names consist of four alphanumeric characters selected by the user. They are used only for identification in the RATCHET log and are not required.

Station position is required and is specified by a pair of numbers that are the distances east and north of the center of the domain in kilometers. Positions west and south of the center are indicated by negative numbers. The stations are not required to be in the model domain.

The wind measurement height is the height, in meters, of the wind instrument above ground. Instrument heights for stations that maintain official records are found in the original station records. Measurement heights may also be found in the *National Wind Data Index* (Changery 1978).

Wind direction and speeds are reported in several different ways. RATCHET can accept and correctly interpret wind directions that are reported using a 16-point compass or in 10-degree increments. It can accept wind speeds measured in miles per hour, knots, or meters per second. However, the user must indicate how the wind data for each station are recorded. This information is included in the meteorological station file in the fields following the surface roughness length. If wind directions are reported in 10-degree increments, enter a 1 in the first of these fields. If they are reported in compass points, enter a 2. Similarly, if wind speeds are reported in meters per second, a 1 should be entered in the second of these fields. If the speeds are reported in miles per hour, enter a 2, and if they are reported in knots, enter a 3.

The status flag is a switch that may be used to eliminate specific stations from consideration in calculating wind fields. The station status must be one if data from the station are to be considered, otherwise the data for the station will be ignored.

3.3.7 Meteorological Station Revision File

Occasionally, meteorological station measurement locations or instrument heights change. RATCHET can adjust the station data to account for these changes as they occur. The changes are entered via a formatted, direct access file called the meteorological station revision file. It is an optional file. These files must be created with a program because they are direct access files. A simple utility program, MAKE_REV, has been prepared to create meteorological station revision files.

The meteorological station revision file contains the same information that is in the meteorological station files plus the date and time of the change. The order of the information in meteorological station revision file records is

- year of the change (last two digits)
- day of the year of the change (three digits)
- hour of the change
- station name (four characters)
- station position (kilometers east/west and north/south)
- wind-measurement height (meters)
- surface roughness length
- wind measurement unit codes (direction and speed)
- station status.

The format for the records is 1X, I2, I3, I2, 1X, A4, 2F10.0, 2F7.0, 1X, 3I4.

The hour of the changes may be difficult to find. If it cannot be found, the change should be assumed to take place at midnight.

3.3.8 Meteorological Data File

The meteorological data file is a direct access, formatted file with a record length determined by the parameter MaxSta that defines the maximum number of meteorological stations that can be used. The number of characters in a record is equal to 18 plus 6 times MaxSta. The file is read in subroutine DATRD. Each time DATRD is called, the file is accessed twice. The first time the file is accessed, the subroutine reads the full data record to obtain data used in transport and diffusion calculations. The second time the file is accessed, the subroutine obtains the date and time of the next set of meteorological data.

A simple utility program, MAKE_MET, may be used to create meteorological data files. Use of a program is required because the meteorological data files are direct access files.

Data are entered in each record in the file in the following order:

- year (last two digits)
- day of the year (three digits)
- hour (two digits)
- release-height wind direction and speed (two digits each)
- release-height temperature (four digits)
- surface-wind direction and speed (two digits each)
- stability class (one digit)
- precipitation code (one digit).

The last three items are repeated for each station. The record must be filled, even if fewer than 25 stations are defined. The utility program uses nines to indicate missing data. The record format is 1X, I2, I3, I2, 1X, 2I2, I4, 1X, 25(2I2, 2I1). The units and ranges for meteorological variables are listed in Table 3.5. The release height temperature is entered as an integer value to the nearest tenth of a degree. RATCHET divides the value entered by 10 when the temperature is converted to degrees Kelvin in subroutine MET_FLD.

3.3.9 Source-Term Data Files

The atmospheric model uses hourly release rate data that are entered via source-term data files. One source-term data file is required for each source defined in the run-specification file. Each record in these files contains a date, time, and release rate. Dates are represented by the year (last two digits) and day of the year (three digits). The time of release is represented by the hour (two digits), and the release rate is the mass or activity released per hour. Hours range from 00 (midnight) to 23 (11 p.m.).

Source-term data files are read by subroutine READQ whenever a change in the source term occurs. The model assumes persistence for each release rate until a different release rate is entered.

Table 3.5. Units and Ranges for Meteorological Variables

Variable	Units	Range
Year	none	00 through 99
Day	none	001 through 366
Hour	none	00 through 23
Release height temperature	0.1°F	none
Wind direction	as defined for Met. Station	00 through 36, 88 and 99
Wind speed	as defined for Met. Station	00 through 80, 88 and 99
Stability class	none	1 through 7
Precipitation class	none	0 through 6

As a result, hourly release rates need to be entered only when the release rate changes. Thus, a uniform release can be entered using two records. The first record gives the time that the release starts and the release rate. The second record gives the time it ends and a release rate of 0.0. Three or more records define a release if additional detail related to the release is available.

Source-term data files are direct access, formatted files having a record length of 21 characters that must be created using a program. They cannot be created or modified using a text editor, but they can be viewed with an editor. The format used to create the file records is 1X,I2,I3,I2,3X,1PE10.3. The file is read using a similar format with E10.3 replacing 1PE10.3.

In the HEDR Project, source-term data files will be provided by the Source Term Task of the HEDR Project. However, it is necessary to create special source-term data files for use in testing the computer code. A simple utility program, MAKE_Q, has been prepared for this purpose.

3.3.10 Residual-Puff Data File

Residual-puff data files provide the means for carrying airborne material within the model domain at the end of a run segment forward to the next segment. They are sequential access, unformatted files that are created automatically at the end of each RATCHET run segment.

The name of one residual-puff data file may be entered via the run-specification file. Entering a name is optional, but if a name is not entered, a blank record must be inserted in place of the name. If a name is entered and the file exists, subroutine PUFFIN will read the file. If a file name is entered and the file cannot be read, the program will abort. The program will continue execution without attempting to read the residual-puff data file when the file name is missing.

Data in the residual-puff data file include the title of the RATCHET run segment that created the file, the date and time of the run creating the file, the number of puffs for which data are recorded, the position and height of the center, the original mass, the last movement, the diffusion coefficients, the depleted mass, a flag, and the source of each puff. The data in the file are in binary form. As a result, the file cannot be examined or modified using a text editor.

3.4 Output Files

RATCHET produces six types of output. They are

- two files containing daily time-integrated air concentrations and surface deposition for use in environmental pathways and dose calculations
- a file providing records of computer-run segments
- an intermediate data file used to pass information from one run segment to the next when several segments are used to cover a period of interest
- a file containing mass-balance summaries for one or more run segments

- a file containing total precipitation summaries for one or more run segments
- a file containing supplementary information on puff status for use in testing model performance.

This section briefly describes the output files.

3.4.1 Time-Integrated Air Concentrations and Deposition

The time-integrated air concentration and surface-deposition files are the primary means of passing information from the atmospheric transport code to the environmental pathways and dose calculation codes. These files are sequential, unformatted files.

One primary output file is created per month for each radionuclide or radionuclide group. This file requires about 500 kilobytes of storage. The name for the primary output file is entered via the twenty-sixth record of the run-specification file. The file begins with a file header record of up to 80 characters. This record is followed by a set of records that contains the daily model output. The general form of the daily model output is

- daily header
- time-integrated air concentrations
- daily header
- surface contamination.

Each daily header record (up to 80 characters) identifies the data that follow and gives the date of simulated and run-segment identification. The data records are binary copies of the model time-integrated air concentration (TICI) and surface-contamination (SCI) arrays.

These arrays have dimensions of 41 (west to east) by 51 (south to north). The spacing between nodes is DELXY/2 in both directions. The binary write of the arrays starts in the southwest corner and writes the array elements from west to east. The rows are written from south to north.

The time-integrated air concentrations in the primary output files are daily accumulations in Ci-s/m^3. They include decay from the time of release to the time of arrival at the grid node. The surface contaminations, which are also daily accumulations, are given in curies per square meter. They include decay during transit and from the time of deposition to midnight at the end of the day of deposition.

A secondary output file is produced by the model primarily for use in model tests. It contains daily time-integrated air concentrations for a nondepositing, nondecaying tracer having the same release characteristics as the actual effluent. The file requires about 250 kilobytes for storage. The name for the secondary output file is entered via the twenty-seventh record in the run-specification file.

These output files are written in a binary format. Text editors cannot be used to read or modify them. A short utility program has been written that may be used to read the files and create

formatted files that can be printed. The utility program is called MONSUM2. The formatted files created by the MONSUM2 are larger than the binary files. They also can be read and modified using a text editor.

3.4.2 Run-Segment Record Files

RATCHET generates a run-log file each time the code is executed. It can also generate a file that contains intermediate computational results.

The RATCHET log file is the primary record of the model run. Its heading lists the program name and version. The log file, which is written to the default output device, has a name derived from the run-specification file name. The first two characters of the log file name are "lg." These characters are substituted for the first two characters of the run-specification file name. The remainder of the run-specification file name is duplicated in the log file name. The log file is an ASCII file that may be viewed or printed.

The log file contains the following information:

- date and time that code execution is begun
- run identification
- fixed model parameters
- input/output file names
- data in run-specification file
- daily mass-balance data
- status and error messages.

If a model run segment terminates in a normal mode, the message

*** SIMULATION TERMINATED ***

is entered in the log. However, this message does not ensure that the model executed as intended. It may have been unable to read one of the optional data files and have simply continued in a default mode. If the program aborts while trying to read a required file, the terminal message in the log will indicate the file access that caused the program to terminate prematurely.

3.4.3 Residual-Puff Data File

RATCHET simulates atmospheric transport and diffusion for long periods by breaking the simulation into segments. The residual-puff data file is used to carry information on material that is airborne in the model domain at the completion of one segment forward to the next segment. For example, the period of interest in the HEDR Project covers many years. Atmospheric transport and diffusion for the full period will not be simulated in a single step. Instead, the code will simulate one month at a time and residual-puff data files will carry information on puff status from one month to the next.

The information to be carried forward in residual-puff data files is primarily related to the position and mass in puffs representing plumes existing at the end of the month. These files are intended for use in subsequent atmospheric model runs. They will not be used by the environmental pathways or dose models.

Subroutine PUFFOUT automatically creates a residual-puff data file each time the code is run. The file is assigned the name entered as the twenty-eighth record. It is an unformatted, sequential access file that cannot be read or modified by a text editor.

3.4.4 Mass-Balance Summary

At the end of each run segment RATCHET will open the file named in the twenty-ninth record of the run-specification file, append two records, and close the file. This file is the mass-balance summary file. If the file named in the run-specification file does not exist, RATCHET will create a file with the name entered.

The first record added to the file describes the period for which the mass balance has been computed. The year, month, day, and hour of the beginning of the run segment are written to the file, followed by the same information for the end of the segment. The second record contains six elements of the mass balance. In order, these elements are

- airborne mass in the model domain at the beginning of the run segment
- mass released during the run segment
- airborne mass transported out of the model domain during the run segment
- airborne mass lost in transit in the domain through radioactive decay
- mass deposited by dry deposition and wet deposition of gases
- mass deposited by wet deposition of particles.

The amount of airborne material in the domain at the end of the run segment is equal to the sum of the first two elements minus the sum of the last four elements. This sum should be equal to the mass in the model domain at the beginning of the next run segment.

3.4.5 Total Precipitation Summary

The file named in the thirtieth record of the run-specification file stores a summary of the total precipitation (water equivalent) at each node of the environmental grid during the run segment. If the named file exists, RATCHET will append the precipitation information to the information already in the file. If the file does not exist, RATCHET will create a file with the name entered.

The primary purpose of the total precipitation summary file is to provide information that can be used to evaluate the performance of the portion of the RATCHET code that estimates precipitation for use in wet deposition calculations. After RATCHET has been run for a month using hourly meteorological data, monthly climatological precipitation records for stations having precipitation records can be compared with the monthly total precipitation predicted by RATCHET. This comparison requires the use of a post-processor code to read the total precipitation summary file and extract the totals for the climatological station locations.

3.4.6 Supplementary Output

If the run identification entered as the first record of the run-specification file has an asterisk as the first character, RATCHET will create a file that contains information that may be used to check intermediate model calculations. The name of this file is created by RATCHET by substituting the letters "ts" for the first 2 characters of the run-specification file name.

RATCHET writes the location and status of all puffs at the end of each hour when this option is selected. The information written includes the puff number, source, status (active or inactive), age in minutes, horizontal position in environmental grid coordinates, transport height in meters, x and y components of the distance moved in the last advection period in meters, diffusion coefficients in meters, initial activity in curies, and remaining activity in curies.

3.5 Program Control

RATCHET is run in a batch mode. User interaction with the code takes place through the run-specification file and other data input files. For simple applications, the executable code and all input files may be moved to a common subdirectory. Then the code can be executed by changing to that subdirectory, typing the name of the executable file followed by the name of the run-specification file on the command line, and pressing the enter key.

Script files can be used to perform a variety of operations and to run the code several times in sequence. Figure 3.18 shows a script file used to run a developmental version of RATCHET for 1945. The first record in the file is a comment that describes the file's purpose and the second record changes the active directory to the directory where the executable code and the unchanging data files reside. The next two records copy the run-specification and source-term files into the active directory. When these steps are complete, the code is executed 12 times in succession. Upon completion of the code execution, the chmod -w command removes write permission from the primary output files. The next set of commands moves the output files to separate directories for storage, and the last two commands delete the run-specification and source-term files that are no longer needed. At the completion of the script, the active directory has been restored to its original status.

Script files of the sort shown in Figure 3.18 can be duplicated, modified, and strung together to permit data processing for long unattended periods. It is also possible to prepare shell scripts that perform the same function with even less intervention by the user. An example of this type of script is included with the code listings, which are available on electronic media from

Technical Steering Panel, c/o K. CharLee
Office of Nuclear Waste Management
Department of Ecology
Technical Support and Publication Information Section
P.O. Box 47651
Olympia, Washington 98504-7651

```
#  SCRIPT 3 FOR DOSE MODEL SENSITIVITY STUDIES  -- 11/19/92
cd /.../rundir
cp /.../rsfiles/*rsf.021  /.../rundir/
cp /.../nov92.q/*q.021  /.../rundir/
ratchet jan45_rsf.021
ratchet feb45_rsf.021
ratchet mar45_rsf.021
ratchet apr45_rsf.021
ratchet may45_rsf.021
ratchet jun45_rsf.021
ratchet jul45_rsf.021
ratchet aug45_rsf.021
ratchet sep45_rsf.021
ratchet oct45_rsf.021
ratchet nov45_rsf.021
ratchet dec45_rsf.021
chmod -w ex* lgf* ng* rpf*
mv pr*  /.../pr_out/
mv ng*.*  /.../ng_out/
mv ex*.*  /.../ex_out/
mv rpf*.*  /.../puffs/
mv *log.*  /.../logs/
rm *rsf.*
rm *q.0*
```

Figure 3.18. Sample Script File that Executes a Sequence of RATCHET Runs

The script in the example performs the following tasks:

- excutes a program to create run-specification files
- copies the meteorological and source-term data files to the subdirectory where RATCHET is to be run
- executes RATCHET for 1945 for realization 21
- distributes the RATCHET output to other subdirectories for storage
- deletes files that are no longer needed.

These tasks are repeated until the requested series of model runs is complete.

3.6 Sample Problems

The two problems presented here may be used for quick checks of the RATCHET code following installation of the code on an new computer. However, neither problem provides a complete

check of the code. A complete check of the code can only be accomplished by running a large number of simple tests that isolate specific code functions, and running one or more tests that cover a period of several months. Both types of tests have been completed during RATCHET development.

The input files and the primary output files for the sample problems are included on the electronic media that contain the code listings for RATCHET and the utility programs. They are available from

Technical Steering Panel, c/o K. CharLee
Office of Nuclear Waste Management
Department of Ecology
Technical Support and Publication Information Section
P.O. Box 47651
Olympia, Washington 98504-7651

3.6.1 Straight-Line Plume Problem

The straight-line Gaussian plume model forms the basis for most regulatory dispersion calculations. Model calculations can be done easily by hand using a scientific calculator. When RATCHET is run with constant release rate, spatially uniform surface conditions, and spatially uniform and temporally constant meteorological conditions, the RATCHET model is equivalent to a Gaussian plume model. Therefore, the first sample problem is one that can be checked using the Gaussian plume model.

The problem is a one-hour elevated release (61 meters) of a reactive gas. The release point is at environmental grid location 8.00,16.75. For meteorological conditions, assume a 10-meters reference height wind from the north at 3 meters per second during neutral stability with a temperature of 35°F. To facilitate model testing, assume that the 200-foot wind data are missing, a constant mixing-layer depth of 2000 meters, and a surface roughness length of 0.1 meters. The release rate is 10 curies per hour. Figure 3.19 shows the run-specification file for the problem. Note that the identification record starts with an asterisk so that test output will be provided.

Table 3.6 contains part of the test output for this problem. The first column lists the puff age (time since release). The second column gives the y-coordinate of the puff. Because the wind is from the north, the x-coordinate of the puff is the same as the x-coordinate of the release point (8.00). The puff positions can be used to test the transport. In this example, the transport should be greater than 3 meters per second because the puff-release height is 61 meters. The log file shows that the 61-meter wind speed is calculated to be 4.18 meters per second; the puff movement for the first hour shows a transport speed of 4.18 meters per second, which is consistent with the 61-meter wind speed. The last two columns give the horizontal and vertical diffusion coefficients at each age. These coefficient values can be compared with hand calculations. They can also be used to calculate time-integrated air concentrations for comparison with model output.

Table 3.7 lists RATCHET results for selected nodes under the centerline of the plume in Sample Problem 1. The values in the table were extracted from the ng_example1 and ex_example1 files

```
* RATCHET  Example 1   North wind @ 3 meters per second, D stability
012745
 0
012745
16
  8000.0
 4
 12
T    1.5
  0
3.72
 1.0E-13
 0.0  0.0
 0.5
Y 2000.0
  44
example1.met
example.sta
(blank record)
(blank record)
example_z0
example.przone
prates.dat
def_mx_h.dat
stab_unc.dat
ex_example1
ng_example1
rp_example1
mbs_example1
mps_example1
 1
 -24.0,      26.0,     61.00
   0.0,      0.0,      0.000
example1.q
    3
    0.
   20.0       30.0000   50.0000
10000.0000    10.0000  100.0000
    0.5000 1000.0000
        0.
        0.
        0.
        0.
        0.
```

Figure 3.19. Run-Specification File for Sample Problem 1

Table 3.6. Partial Test Output for Sample Problem 1

Puff Age (min)	Y Posit. Env. Grid	σ_y (m)	σ_z (m)
0	16.75	0	0
15	16.28	145.1	290.1
30	15.81	290.1	580.2
45	15.34	435.2	870.3
60	14.87	580.2	1160.
75	14.40	1030.	1451.
90	13.93	1480.	1600.
120	12.99	2380.	1600.
150	12.05	3280.	1600.
180	11.11	4180.	1600.
232.5	9.46	5755.	1600.
277.5	8.05	7105.	1600.
337.5	6.17	8905.	1600.
397.5	4.29	10,710.	1600.
457.5	2.41	12,510.	1600.
517.5	0.53	14,310.	1600.

Table 3.7. RATCHET Results for Selected Nodes for Sample Problem 1

Conc. Grid Y Coord.	Time-Integrated Air Noble Gas	Particles	Surface Contamination
32	5.9E-5	5.7E-5	3.4E-7
31	7.0E-6	6.7E-6	4.0E-8
30	2.6E-6	2.4E-6	1.4E-8
29	1.3E-6	1.2E-6	7.3E-9
28	5.7E-7	5.3E-7	3.2E-9
27	3.5E-7	3.3E-7	1.9E-9
26	2.2E-7	2.0E-7	1.2E-9
25	1.8E-7	1.7E-7	1.0E-9
24	1.6E-7	1.5E-7	9.0E-10
23	1.4E-7	1.3E-7	7.8E-10
22	1.3E-7	1.2E-7	6.9E-10
21	1.1E-7	1.0E-7	6.0E-10
20	9.7E-8	8.9E-8	5.3E-10
18	8.4E-8	7.7E-7	4.6E-10
16	7.5E-8	6.8E-8	4.0E-10
14	6.3E-8	5.7E-7	3.4E-10
12	5.6E-8	5.0E-8	3.0E-10
10	5.0E-8	4.5E-8	2.6E-10
7	4.3E-8	3.9E-8	2.3E-10
4	3.8E-8	3.4E-8	2.0E-10
1	3.4E-8	3.0E-8	1.8E-10

created by RATCHET using the MODSUM2 utility program. Remember that the spacing of RATCHET output is equal to half the spacing specified in the run-specification file.

3.6.2 Box-Transport Problem

The second example problem is designed to check transport calculations with temporally varying wind directions. The model domain, release location, and release rate and duration are the same as in the previous example. Figure 3.20 shows the run-specification file for this example.

```
* RATCHET  Example 2   Box Pattern @ 4 meters per second, D stability, Precip
on 2nd leg
012745
 0
012745
16
  8000.0
 4
 12
F
  0
3.72
 1.0E-13
 0.0  0.0
 0.5
Y 2000.0
  44
example2.met
example.sta
(blank record)
(blank record)
example_z0
example.prz1
prates.dat
def_mx_h.dat
stab_unc.dat
ex_example2
ng_example2
rp_example2
mbs_example2
mps_example2
 1
 -24.0,      26.0,     61.00
   0.0,      0.0,      0.000
example1.q
    4
    0.
   20.0       30.0000   50.0000
10000.0000    10.0000  100.0000
    0.5000 1000.0000
        0.
        0.
        0.
        0.
        0.
```

Figure 3.20. Run-Specification File for Sample Problem 2

The meteorological conditions defined in example2.met are as follows. For the first four hours, the wind direction and speed are north at 4 meters per second. At the beginning of the fifth hour, the wind direction changes from north to west, and light rain begins. These conditions persist for 4 hours. At the beginning of the ninth hour, the rain stops and the wind direction shifts to south. Finally at the beginning of the thirteenth hour, the wind direction changes to east. Assume D stability, a 35.0 °F temperature, and missing 200-foot winds as before.

Assuming that the final wind direction persists for at least four hours, the first puff will pass over the release point 16 hours after it was released. Table 3.8, abstracted from the test output file, shows the position and mass in the first puff each hour. Note that the puff does, in fact, return to its release point at the end of the sixteenth hour. Comparison of the puff depletion rate during the periods before and after the precipitation with the rate during precipitation shows a significant change.

Table 3.8. Puff Position and Mass in Sample Problem 2

Puff Age (hr)	Env. Grid X Coordinate	Env. Grid Y Coordinate	Depleted Q
0	8.00	16.75	2.500
1	8.00	14.24	2.380
2	8.00	11.74	2.345
3	8.00	9.23	2.311
4	8.00	6.72	2.277
5	10.51	6.72	1.976
6	13.01	6.72	1.714
7	15.52	6.72	1.487
8	18.03	6.72	1.290
9	18.03	9.23	1.271
10	18.03	11.74	1.252
11	18.03	14.24	1.234
12	18.03	16.75	1.216
13	15.52	16.75	1.198
14	13.01	16.75	1.181
15	10.51	16.75	1.164
16	8.00	16.75	1.147

Table 3.9 contains the results of RATCHET calculations for selected nodes. Again the MONSUM2 utility program was used to extract the node values from the binary RATCHET output files. The nodes tend to follow the path of the first puff released. However, only the nodes on the first leg (x-coordinate = 15) are under the plume centerline. During the west and east winds, the

Table 3.9. RATCHET Results for Selected Nodes for Sample Problem 2

Concentration Grid Position (x,y)	Time-Integrated Air Concentrations		
	Noble Gas	Iodine-131	Surface Contamination
15,32	4.3E-5	4.2E-5	3.4E-7
15,26	2.6E-7	2.4E-5	1.9E-9
15,20	1.0E-7	9.5E-8	7.9E-10
15,14	4.9E-8	4.4E-8	1.3E-9
20,14	3.7E-8	3.0E-8	2.3E-9
25,14	3.3E-8	2.3E-8	1.8E-9
30,14	3.1E-8	1.9E-8	1.3E-9
35,14	2.5E-8	1.4E-8	6.9E-10
35,23	2.4E-8	1.2E-8	1.1E-10
35,32	2.1E-8	1.0E-8	8.3E-11
30,32	1.9E-8	9.1E-9	7.5E-11
25,32	1.4E-8	6.4E-9	5.2E-11
20,32	1.0E-8	4.8E-9	3.9E-11

four puffs are moving across the grid in a line that resembles a flanking movement in marching. As a result, the nodes selected do not have the highest values.

Note that ratios of the values in the Surface-Contamination column to the Time-Integrated Air Concentration values in the second and third columns can be considered to be effective deposition velocities. These ratios provide another indication of the effect of precipitation on deposition.

4.0 Programmer's Guide

Chapter 2 discussed the technical basis for the RATCHET computer code. The last chapter discussed the computer code from a user's point of view. This chapter discusses the code from a programmer's point of view. It covers programming style, hardware requirements of the code, and the individual program elements.

The RATCHET computer code was written to meet the following general goals:

- the models used should be appropriate for the questions being addressed in the HEDR Project
- the process models and model input should be technically defensible
- the computer codes implementing the models should not require more than 1 second of computer time per hour simulated.

Elaborate steps have been taken to ensure that these goals are met by the code.

The first goal was addressed in the model-selection process. Ramsdell (1991) discussed the practical alternatives for transport and dispersion modeling and recommended a Lagrangian-trajectory, Gaussian- puff modeling approach. The feasibility of the approach was demonstrated in the early phase of the HEDR Project (Ramsdell and Burk 1991a, 1991b). A TSP review[(a)] following the initial model calculations determined that the basic atmospheric modeling approach was appropriate. However, analysis of the results of the calculations (Simpson 1991a, 1991b) indicated that substantial modeling changes in the basic approach were required. The code documented here incorporates the changes directed by the TSP.

The second goal was addressed in the selection of components for use in revising the early HEDR atmospheric model. The TSP directed that a Monte Carlo modeling approach be used to estimate the effects of uncertainty on model predictions. A working group meeting was convened in March 1991 to consider representation of atmospheric processes in the transport and diffusion model (Ramsdell 1992). The group's recommendations on models for various processes included an internally consistent set of equations representing atmospheric processes. To a large extent, those recommendations have been implemented. The working group recommendation related to elevated winds has not been implemented because data on upper-level winds are not available during the period of the largest releases. Several alternatives to the use of upper-level wind data, including arbitrary rotation of wind directions and estimation of upper-level winds from surface pressures, have been considered and rejected (Ramsdell and Skyllingstad 1993). The lack of upper air data also resulted in deviation from the group recommendations related to calculation of the mixing-layer depth. Technical bases for other revisions to the atmospheric transport model are addressed in Section 2.

(a) Unpublished Report (HEDR Project Document No. 01910072), "Atmospheric Transport and Diffusion Modeling (ATDM) Workshop (Richland, WA; June 12-13, 1990) Summary Report," from A. H. Murphy (HEDR Technical Steering Panel) to the HEDR Technical Steering Panel, Washington State Department of Ecology.

The third goal was addressed as the code was developed. Section 3.2 includes a discussion of code tests conducted to ensure that measures taken to reduce run time did not adversely affect code accuracy. In October 1993, calculations were made for a set of 100 realizations of the period between December 26, 1944 and the end of December 1949. The calculations covered a period of almost 4,400,000 hours and took almost 296 hours of computer time. This amounts to about 0.24 seconds of computer time per hour simulated. The third goal has clearly been met.

4.1 Program Development

This section discusses three components related to program development: programming language and style, the hardware for which the program was developed, and the size of the program and its files.

4.1.1 Language and Style

RATCHET is written in standard ANSI FORTRAN-77 programming language with extensions designed to enhance code maintenance and to promote a structured programming style. Specific extensions used include long variable names, IMPLICIT NONE, INCLUDE statements, and the DO WHILE and END DO statements.

In addition to formatted, sequential files, the code makes use of formatted, direct access files and unformatted, binary data files. These files are computer specific, but the read and write statements for the files follow the ANSI standard, except as noted above. The code also uses three computer-specific subroutines. One subroutine is used to read the command line argument that specifies the name of the run-specification file and the other two subroutines obtain the current date and time from the system clock.

The following coding standards are followed in the program:

- The code for each program unit includes a definition block and a code block. The definition block includes the program unit name, history, description, and relationship to other units and INCLUDE files. It may also contain references, describe algorithms, and define variables. The code block contains the code and comments.

- All program units begin with the statement IMPLICIT NONE. The type and dimensions of all variables are defined in type statements.

- Named common blocks are the primary method of passing variables between major program units. They contain generally related information with the block names indicating the general nature of the information. The common blocks are defined in code segments contained in INCLUDE files. INCLUDE files also contain PARAMETER statements, type definitions, and dimensions associated with all variables in the common blocks defined in the file.

- Functions are used in preference to subroutines when possible. Common blocks are not used to pass variables to functions.

- Argument lists are used to pass variables to functions and to some subroutines. The use of formal argument lists is preferred in functions and in subroutines where the formal argument list facilitates program development, verification, and maintenance.

- Parameter statements are used to define array dimensions that establish the model domain size and model limits. All of these statements are located in the PARM.INC file.

- Data statements used to define variables contained in common blocks are placed in the BLOCK DATA unit. The code for the BLOCK DATA unit is located at the end of the code for the main program.

- Use of system-dependent calls has been minimized. They have been limited to the calls to the system clock to determine the date and time of program execution.

- Structured programming techniques (IF...THEN, ELSE IF... THEN, DO WHILE) have been used when appropriate. The use of statement numbers has been minimized.

RATCHET includes its own random-number generator. The random-number generator is described in Section 4.3.7.

4.1.2 Target Computer

RATCHET is implemented on RISC/SPARC-based hardware using a UNIX or UNIX-based operating system. However, much of the code development and testing has taken place on personal computers and on a VAX 6000 series computer system. The code has been compiled and run on various Sun computers using versions 4.1.2 and 4.1.3 of the SunOS operation system. The code has also been ported to, modified for, and run on personal computers using version 5.1 of the MS-DOS operating system. The PC version of RATCHET has not been tested and is known to contain errors.

Input data required by RATCHET have been obtained from many sources, entered into flat files, and documented. The input files and their documentation are included in the HEDR Project records.

The meteorological data and RATCHET output files may be converted into files suitable for use with a geographic information system. This conversion involves reading the files using a post-processing program with appropriate read formats and rewriting the files in a format compatible with the specific geographic information system in use. This document does not include a post-processing program for this purpose.

4.1.3 Program Size

RATCHET is a sufficiently small program to fit within the memory limits of personal computers. However, RATCHET processes data one month at a time and produces daily output. As a result, several of the files used and created by the program are relatively large. Monthly meteorological data files exceed 100 kb, and monthly output may exceed 900 kb.

4.2 Program Organization

RATCHET is a highly modular code consisting of a main program and block data element, 26 subroutines, and 19 functions. In addition, there are 10 INCLUDE blocks that contain parameter, type, and common statements. The main program provides a general framework for the code and controls the sequence of code execution. The subroutines and functions perform most of the calculations.

The following sections describe the main program and the other program units.

4.2.1 Main Program

The main program provides the general framework for the code. It contains the six sections listed below:

- an initialization section
- an hourly environment and source-update section
- a transport, diffusion, and deposition-calculation section
- an hourly and daily output section
- a housekeeping section
- a program-termination section.

Figure 4.1 shows the general organization of these parts.

The initialization section determines the date and time of code execution, opens the run-log file, and controls model initialization. Code initialization begins by calling a subroutine that reads the run-specification file containing user input. Then, additional subroutines read data files that contain initial conditions and default data.

When initialization is complete, the code enters an hourly loop that performs the model computations. This loop contains the hourly environment and source-update section; the transport, diffusion, and deposition-calculation section; the hourly and daily output sections; and the housekeeping section.

The transport, diffusion, and deposition section of the code involves two nested loops. The outer loop has a time-increment determined by the variable NPH, which is supplied by the user. The time increment in minutes is 60/NPH. This increment is referred to as the advection period. The loop starts by generating new puffs if there are active sources. After a new puff is generated for each active source, the code enters the inner loop. In this loop, each puff is moved, and diffusion and deposition calculations are made. The time step used in puff movement and the diffusion and deposition calculations is called the sampling interval. It depends on puff size. Calculations for small puffs may be made at 1-minute intervals. As puffs grow, the time step increases until a maximum time step is reached. The maximum time step is the interval between puff releases (1/NPH hours).

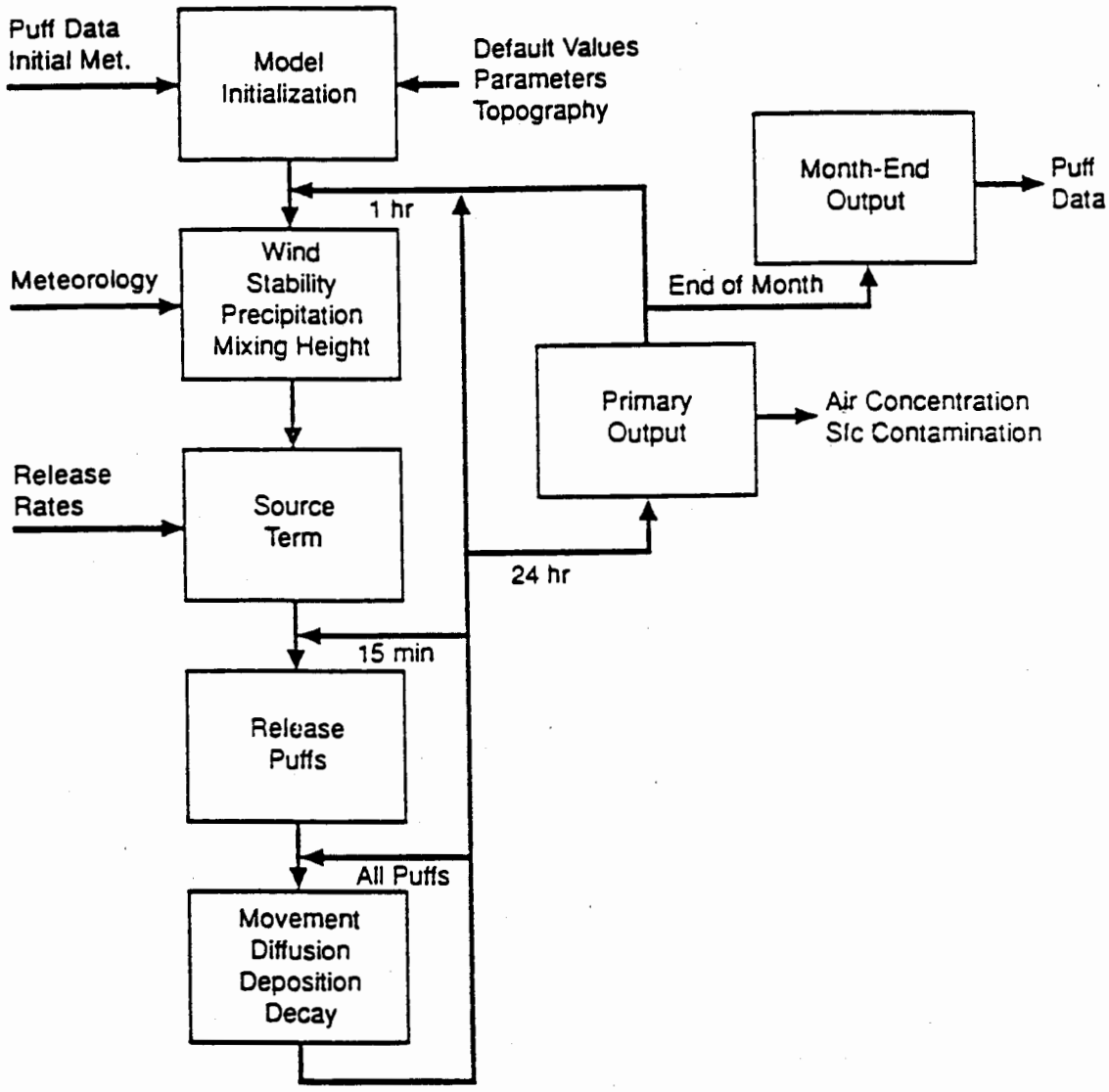

Figure 4.1. Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET)

After the transport, diffusion, and deposition calculations have been completed, the code enters the hourly and daily output section. The primary code output is written to files at the end of each day. This output consists of sets of daily time-integrated air concentrations for depositing and nondepositing material, and surface contamination for depositing material. At the end of each day, the code also performs a set of mass-balance calculations and records the results on the program run log. If the code-testing mode has been selected, an additional file will be created. This file contains hourly test output. The test output includes the status, position, dimensions, movement, and mass of each puff during the last advection period of the hour.

Each hour, the code enters the housekeeping section in which the status of the puffs is examined. Puffs that have moved out of the model domain or have been depleted so that the concentrations in the puffs are negligible are deleted. The *de minimis* concentration entered by the user is used as the basis for determining if a puff within the model domain may be deleted. The positions and dimensions of consecutive puffs from the same source are also examined. If the separation between puffs is small compared to their size, the puffs are combined into a single puff and one puff is deleted.

The code leaves the hourly loop when the time specified in the run-specification file for terminating the model simulation is reached. It then enters the termination section. This section of the code saves information on active puffs within the model domain for future model runs, writes a message indicating normal model termination, and closes files as appropriate.

4.2.2 Relationships Between Program Units

The section just completed gives a general overview of the structure of RATCHET. This section provides more detail on the interrelationships between the program units. The next section contains a description of each of the units.

The subroutine calling sequence in RATCHET is shown in Figure 4.2. Nineteen of the program's 26 subroutines are called by the main program. The main program sections are indicated by mixed upper- and lower-case headings. Subroutine names are shown in upper-case letters, and the indentation indicates the level of nesting of the subroutines. The comment to the right of the subroutine name gives an indication of the subroutine's purpose.

Data are generally passed between subroutines using named common blocks. These common blocks are defined in INCLUDE files that are incorporated in the code of subroutines as the subroutines are compiled. In addition to the common block definitions, the INCLUDE blocks contain type statements and, where needed, parameter statements. All variables in the common blocks are included in type statements. Table 4.1 shows the INCLUDE files associated with each subroutine.

Nineteen special-purpose functions have been developed for use in RATCHET. Most of these functions are used to calculate variables used in the transport, diffusion, and deposition calculations. Special functions have also been developed for use in time conversions within the program and for random sampling. None of these functions use INCLUDE files; all data are passed to the functions via formal argument lists. Table 4.2 shows a list of the RATCHET functions used in each subroutine.

4.3 Program Element Descriptions

The last section discussed the main program and the relationship between program elements. This section describes each of the remaining program elements. The subroutines are discussed first in groups related to their functions in the overall program. The subroutines in each group are listed alphabetically. The functions are discussed in alphabetical order following the descriptions of subroutines.

```
RATCHET
Model Initialization Section
    GETARG  -- get command line arguments (system)
    IDATE   -- get current date (system)
    SPECIN  -- read run-specification file
    PUFFIN  -- read residual-puff data file, if specified
    GRIDIN  -- initialize computational grid
        STRAY-- associate nodes with met. stations
            ASCND-- sort station list by distance from node
        READ_STA-- update station locations, if required
            STRAY
            ASCND
    INIT    -- set up initial met. conditions
        METOPN-- find initial met. record in file
        DATRD-- read met. data
        DATWR-- write first met. data record to log file
        MET_FLD2-- decode met. data, set up met. fields
            DATACK-- check met. data for availability
            SUBST200-- substitute HMS 200' winds for surface winds
            REG2D-- fit plane to station mixing height estimates
    RELEAS  -- initialize source term
Hourly Environment and Source-Update Section
    READ_STA
        STRAY
            ASCND
    DATRD
    MET_FLD2
        DATACK
        SUBST200
        REG2D
    READQ   -- read source-term data file
Diffusion and Deposition Calculation Section
    PUFFR   -- assign puff attributes at release time
    PUFFM   -- compute puff movement
    DIFDEP  -- diffusion, deposition, decay and depletion
Hourly and Daily Output Section
    BALANCE -- daily mass-balance calculation
    OUTPUT  -- output daily results
    TESTM   -- output info. on puffs, if requested
Housekeeping Section
    COMBINE -- combine overlapping puffs, if requested
    CLEAN2  -- delete inactive puffs
Month-end Output Section
    FBALANCE-- output cumulative mass balance
    PUFFOUT -- create residual-puff data file
```

Figure 4.2. The RATCHET Subroutine Call Sequence

4.3.1 Initialization Subroutines

The following nine subroutines are used primarily in the initialization phase of RATCHET. Several other subroutines, for example DATRD and MET_FLD2, are used in the initialization phase but are called hourly. These subroutines are discussed later.

Table 4.1. Cross Reference between Subroutines and INCLUDE Files

	INCLUDE FILE									
	CONST	DATES	MASS_BAL	MATRIX	MET_DATA	PARM	PUFFS	RAND_DAT	REL	STATION
RATCHET	X	X	X	X	X	X	X	X	X	X
BLOCKDATA	X			X	X	X	X			
ASCND						X				X
BALANCE		X	X	X		X	X			
CLEAN2	X	X				X	X			
COMBINE	X	X				X	X			
DATACK					X	X				X
DATRD		X			X	X				
DATWR		X			X	X				
DIFDEP	X	X	X	X	X	X	X		X	X
FBALANCE			X							
GRIDIN	X	X	X			X				X
INIT	X	X	X		X	X	X			X
MET_FLD2	X	X			X	X		X		X
METOPN		X				X				
OUTPUT		X		X		X				
PUFFIN			X			X	X	X		
PUFFM	X	X			X	X	X		X	X
PUFFOUT		X				X	X	X		
PUFFR		X	X		X	X	X		X	
READ_STA	X	X				X				X
READQ		X				X			X	
REG2D						X				
RELEAS	X	X				X			X	
SPECIN	X	X	X	X	X	X	X	X	X	X
STRAY					X	X				X
SUBST200					X	X				X
TESTM	X	X				X	X			

Subroutine ASCND

Subroutine ASCND is a bubble-sort routine. It arranges the distances in a node-to-station distance vector in order of increasing magnitude. The order of the station numbers is adjusted as the order of the distances is adjusted to maintain the correspondence between station numbers and distances.

Subroutine ASCND is called from subroutine STRAY any time a change is made in the meteorological station data.

Subroutine DATWR

Subroutine DATWR writes the initial meteorological data record to the RATCHET log. It provides a check to ensure that the meteorological data file is being read correctly. DATWR is called from subroutine INIT after subroutine DATRD reads the first meteorological record and before the subroutine MET_FLD2 is called.

Table 4.2. Cross Reference between Subroutines and RATCHET Functions

SUBROUTINE	FUNCTIONS USED
RATCHET	MXLD_EST, PLUMRISE
ASCND	None
BALANCE	HOURDT
CLEAN2	None
COMBINE	None
DATACK	None
DATRD	DTHOUR
DATWR	None
DIFDEP	DDEPVEL, MXLD_EST, PUFFSIGZ, PUFSIGY, TURBSIGV, TURBSIGW, USTAR, WDEPGAS, WDEPPART
FBALANCE	None
GRIDIN	DTHOUR
INIT	None
MET_FLD2	HOURDT, INVMOL, MIX_HT, PRCPRATE, PROFILE, RAN_STAB, USTAR, U01
METOPN	DTHOUR
OUTPUT	HOURDT
PUFFIN	None
PUFFM	PROFILE, USTAR
PUFFOUT	None
PUFFR	None
READ_STA	DTHOUR
READQ	DTHOUR
REG2D	None
RELEAS	DTHOUR
SPECIN	DTHOUR, JULIAN
STRAY	None
SUBST200	PROFILE, USTAR
TESTM	HOURDT

Subroutine GRIDIN

Subroutine GRIDIN sets up the model domain. It reads the surface roughness length, precipitation regime, and meteorological station files. If a meteorological station revision file name has been entered, GRIDIN will compare dates of meteorological station changes in the station revision file with the starting date of the run segment and make any needed changes in station information. Finally, it records data related to the model domain in the RATCHET log file.

GRIDIN determines the position of the meteorological stations in environmental grid coordinates from the distance components in the meteorological station file and the node spacing. When the meteorological station positions have been defined, the subroutine deletes any stations that are marked as inactive. It then calls subroutine STRAY, which builds a look-up table for each node that gives the distance from the node to each meteorological station. STRAY, in turn, calls subroutine ASCND, which arranges the entries in the look-up table in order of increasing distance.

GRIDIN records information about the model domain and meteorological station in the log file. This information includes the number of nodes along each axis, the center of the model domain, and the spacing between nodes on the environmental grid. It lists the environmental grid coordinates, wind-measurement height, surface roughness length, wind-unit codes, and status for each station. Following the list of meteorological stations, GRIDIN writes arrays showing the station numbers for the three meteorological stations closest to each node. Finally, it calculates and records the area associated with each node on the concentration grids.

Subroutine INIT

Subroutine INIT is the primary initialization routine for diffusion and deposition calculations. It starts by checking to ensure that the number of puffs to be released each hour entered via the run-specification file is an integer factor of 60. If it is not, program execution will be aborted. INIT then initializes the puff counter and the variables used in the mass-balance calculations.

INIT then reads three data files required for model execution. These files are the surface roughness length file, the default mixing-layer depth file, and the stability class cumulative frequency distribution file. Names for these files are entered via the run-specification file. The surface roughness length array is written to the log file.

The subroutine then performs meteorological initialization, which includes 1) calling subroutine METOPN to find the initial meteorological data record for the simulation, 2) calling subroutine DATRD to read the initial meteorological data, 3) calling subroutine DATWR to copy the initial meteorological data record to the RATCHET log, and 4) calling subroutine MET_FLD2 to process the initial meteorological data set. The initial stability and precipitation fields are written to the log file along with the mixing-layer depths calculated for each station. The log file also contains the results of the regression that fits a plane to the mixing-layer depths to describe their spatial variation for use in model calculations.

When the meteorological data initialization is complete, INIT records the run title, date, and time on the log. If the additional output for use in code verification has been requested, a note to that effect is written. Finally, INIT records the time that the simulation is to start on the RATCHET log.

Subroutine METOPN

Subroutine METOPN is used to open the meteorological data file and to set the meteorological record index to the proper set of observations for the start of the simulation. If the character variable METFILE does not contain the name of a meteorological data file, if there is an error in opening the

file, or if an error is encountered in reading the date/time group in the first record, METOPN will write a message to the RATCHET log that identifies the problem. It will then abort execution of the program.

After the date/time group in the first record has been read successfully, an error in reading a subsequent date/time group will result only in writing an error message to the log. The simulation will continue. Data will be used as appropriate until the record in which the error occurred is encountered. The remainder of the simulation will use the data in the last good record.

Subroutine PUFFIN

Subroutine PUFFIN reads in the residual-puff data file, if one exists. The name of the residual-puff data file is entered via the run-specification file. When PUFFIN is called by RATCHET, the subroutine immediately checks the residual-puff data file name and returns to the main program if the name is blank. If the name is not blank and the file cannot be opened, program execution is aborted. If the file can be opened, PUFFIN reads it.

After the residual-puff data file is read, PUFFIN computes the amount of airborne material in the model domain at the beginning of the run segment. This information is used later in mass-balance calculations.

Prior to returning to the main program, PUFFIN records three items in the RATCHET log file. These are the number of puffs for which data were read, the heading of the residual-puff data file, and the date and time of the run segment that created the residual-puff data file. It then writes five random-number seeds from the previous run segment. These seeds are used in place of the seeds entered in the run-specification file.

Subroutine RELEAS

Subroutine RELEAS has three functions. It checks the source-term data files, determines release rates for the start of the run segment, and defines and checks the positions of the sources.

RELEAS checks to ensure that a source-term data file exists and can be opened for the number of sources specified in the run-specification file. If there is an error in opening any of the source-term data files, program execution is aborted.

While each source-term data file is open, RELEAS determines the date and time of the first record in the file. After all files have been checked, RELEAS enters a DO WHILE loop in which it first finds the last record in each file for a time prior to the start of the run segment, then determines the release rate for the source at the beginning of the simulation.

Subroutine RELEAS then defines the position of the sources. In general, RATCHET has the ability to treat simultaneous releases from four sources. The releases may be from any location within the model domain, and from any release height from the ground to 300 meters. The position of the sources is recorded on the RATCHET log. If any of the positions are out of the model domain or are greater than 300 meters, program execution will be aborted.

The release schedule is established using the time information in source-term data files.

Subroutine SPECIN

Subroutine SPECIN has two primary functions. It reads the run-specification file, and it records much of the run-specification file information in the RATCHET log file. The run-specification file is discussed in detail in Section 3.1. If SPECIN cannot open the run-specification file, program execution will be aborted.

SPECIN does not perform any calculations. However, it does call functions JULIAN and DTHOUR to convert dates and times entered by the user to internal model times. The internal model time is elapsed time from midnight beginning the first of January of the reference year supplied by the user in the run-specification file. SPECIN also sets five logical flags that are used to control random sampling in the model. These flags are initially set .TRUE. The initial random-number seeds in the run-specification file are checked, and flags are reset .FALSE. for each option that has a zero seed.

Subroutine STRAY

Subroutine STRAY sets up two three-dimensional arrays that relate the meteorological stations to the nodes on the environmental grid. One of these arrays contains the distance from each node to each meteorological station, and the other array contains identification numbers assigned to the meteorological stations. The distances in the first array correspond to the station identification numbers in the second.

The data for each node are initially entered into two vectors. STRAY calls subroutine ASCND to arrange the station data in the two vectors in order of increasing distance. After the order of the data has been established, the data are copied into the final three-dimensional distance and station number and arrays.

4.3.2 Hourly Update Subroutines

The seven subroutines discussed in this section are used by RATCHET to update model status each hour. Four of the subroutines are called directly by the main program. They are READ_STA, DATRD, MET_FLD2, and READQ. MET_FLD2 calls DATACK, SUBST200, and REG2D.

Subroutine DATACK

Subroutine DATACK screens meteorological data records for valid wind, stability, and precipitation data prior to data processing in Subroutine MET_FLD2. The results of the screening are stored in the logical variables windck, stabck, and precipck, which are returned to MET_FLD2.

The upper-level wind data are checked first, then the surface data are checked. After one valid wind data point is found, windck is set to .TRUE. Further checking of wind data is bypassed. A similar process is followed for stability and precipitation data.

Thus, all that .TRUE. logical variables indicate is that there is at least one valid value of the type in the current record. This is sufficient to prevent MET_FLD2 from replacing an hour-old field based on data with a field that has no data. In fact, an hour-old data field based on 10 or 12 data points may be better than a current field based on one or two data points.

Subroutine DATRD

Subroutine DATRD is used to read formatted records from the direct-access meteorological data file. METOPN reads date/time groups until it identifies the record containing the meteorological data to be used at the beginning of a simulation. The variable MINDEX contains the number of that record. When DATRD is called, it reads the complete record identified in MINDEX.

If an error occurs in reading the data, the record number and error condition are written to the RATCHET log. The simulation will continue using the last meteorological data read without error.

If the data record is read successfully, DATRD attempts to read the date/time group of the next record. If the attempt is successful, the date and time are converted to a time that is used to trigger the next meteorological data read, and MINDEX is incremented by 1. If an error occurs in reading the date/time group, the error is noted in the log, and an end-of-file flag is set for the meteorological data. In either case, the simulation will continue with the last set of meteorological observations that were read successfully.

Subroutine MET_FLD2

Subroutine MET_FLD2 processes the meteorological data each hour. It decodes wind, stability, and precipitation data from the meteorological stations; adjusts wind speeds to a common 10-meter reference height; and generates the wind, stability, precipitation, and mixing height fields. All random sampling related to uncertainty in the meteorological data occurs in MET_FLD2.

The first stage in processing the meteorological data is to check the station data read by subroutine DATRD. In this stage, DATACK is called to determine status of the meteorological data in the current record. Three logical variables—windck, stabck, and precipck—are used to indicate the status of wind, stability, and precipitation data, respectively. If the logical variables are .FALSE., the record does not contain good data. When a record does not contain good data, persistence is assumed and the previous field is reused. A note is written to the log any time persistence is used. If the variables are .TRUE., the record contains data and data processing continues.

Decoding of the meteorological data record is the next stage of data processing. Wind speeds are converted from the units in which they were recorded to meters per second, and wind directions are converted to degrees. Random sampling of winds, if selected, takes place just prior to the unit conversion. Stabilities are decoded and inverse Monin-Obukhov lengths are calculated. Random sampling related to stability takes place in this stage, if selected. Precipitation classes are decoded, and the precipitation rate is selected if precipitation is occurring. At the completion of the decoding stage, all of the valid meteorological data for each station are ready for use in preparation of meteorological fields.

Following the decoding of the meteorological data, MET_FLD2 generates the stability and precipitation class fields. Stability and precipitation classes are estimated for each node on the environmental grid. In both cases, the values used for each node are the reported values for the meteorological station closest to the node that has valid data.

When the stability and precipitation fields are completed, the subroutine returns to the station winds. All wind speeds measured at heights below 8 meters or above 12 meters are adjusted to a reference height of 10 meters using the diabatic wind profile. In this process, MET_FLD2 uses the INVMOL, USTAR and PROFILE functions. Wind speeds measured at heights between 8 meters and 12 meters are not adjusted. At this time, MET_FLD2 also determines the mixing-layer depth using the MIX_HT function. If a station wind is calm or the wind speed is missing, the estimation of mixing-layer depth is bypassed.

Following adjustment of the wind speeds and determination of mixing-layer depths, MET_FLD2 calls subroutine SUBST200 to substitute a 10-meter wind estimated from the upper-level wind data for the surface data for the first meteorological station. This process ensures that the release-height wind controls the dispersion of material near the release point. It is a substitution that is made specifically for the HEDR Project.

When the substitution is complete, the MET_FLD2 computes the "u" and "v" components of the transport vector at each station. A positive "u" indicates transport to the east, and a positive "v" indicates transport to the north.

Transport components at nodes on the environmental grid are then computed by weighted interpolation. The interpolation weights are inversely proportional to the square of the distance between the meteorological station and the node. Only the data from the closest meteorological stations are used for the interpolation. The maximum number of locations considered in the interpolation is five. If data are available from fewer than three locations, all data are used in the interpolation regardless of distance. If meteorological data are available from three or more locations, the data from the closest two stations are used regardless of distance, but the data from the next three stations are used only if the stations are within 80 kilometers of the node.

The next stage in processing the meteorological data is to determine the spatial variation of the mixing-layer depth. RATCHET has two options related to mixing-layer depth—a spatially varying depth and a constant depth. If the option for a spatially varying mixing-layer depth is selected in the run-specification file, MET_FLD2 calls subroutine REG2D, which fits a plane to the station mixing-layer depths. If the option for constant depth is selected, the constant value specified by the user is substituted for the mixing-layer depth determined for each station prior to calling REG2D. In either case, the output from REG2D is used to determine mixing-layer depths for the hour.

In the final stage for processing meteorological data, the ambient air temperature is converted from degrees Fahrenheit to degrees Kelvin. When this step is complete, MET_FLD2 returns to the calling program.

Subroutine READQ

Subroutine READQ reads source-term data from a formatted, direct access file. READQ is called from RATCHET. The source number is passed to the subroutine and the source term is returned to the calling program unit via formal arguments. The file names are passed via common blocks defined in the INCLUDE statements.

Each time it is called, READQ opens the source-term file and reads two records. The first record is read to obtain the new source term, and the second is read to get the date and time of the next source-term change. READQ uses the DTHOUR function to convert the date and time of the next change to a time relative to the model reference. The time of the next change is stored in the variable TOTHR_NEXTQ. The record number for the data is stored in the variable QINDEX.

Subroutine READ_STA

Subroutine READ_STA is used to read meteorological station revision files. Each time the subroutine is called it reads two records. The first record is read to obtain revisions to meteorological station information and the second to determine the time of the next revision. READ_STA uses the DTHOUR function to convert dates and times to the model internal times.

After the revised station information has been read, the subroutine determines the station number to which the revision applies, makes the revision, and calls subroutine STRAY to revise the node-to-station distance arrays. The revised station information is noted in the RATCHET log file.

Subroutine REG2D

Subroutine REG2D is a general-purpose, linear-regression routine used to fit a plane to variables in two dimensions. It is used to calculate the coefficients for the equation of a plane that best represents the spatial variation of the mixing-layer depth.

The procedures for determining the regression coefficients and evaluating the significance of the regression are described by Snedecor and Cochran (1980). If there are fewer than five meteorological station mixing-layer depths or the regression is not significant at the 10-percent level, the subroutine returns the average mixing-layer depth rather than the regression coefficients.

The subroutine returns the sums, sums of squares, and sums of products that were used to compute the regression. However, these values are not used or stored by RATCHET. They are included in the data returned to facilitate testing of the subroutine.

Subroutine SUBST200

Subroutine SUBST200 is used to ensure that the 200 foot-level winds will be used in calculating the initial transport and dispersion of effluents from fuel-separation facilities at the Hanford Site. If the 200 foot-level winds are good, the wind direction is substituted directly for lower direction and the speed is adjusted to the 10-meter level and substituted for the lower speed.

SUBST200 performs a second function. If the wind observations at the 200-foot level and at the surface for the first station are incomplete, the subroutine will attempt to put together a composite observation for the first station from the available direction and speed information.

4.3.3 Transport and Diffusion Subroutines

Three subroutines are directly involved in the atmospheric transport and diffusion calculations. These subroutines are PUFFR, PUFFM, and DIFDEP. PUFFR creates the puffs; PUFFM computes puff movement; and DIFDEP moves the puffs, computes their diffusion, computes the time-integrated air concentrations and surface contamination, and makes corrections for puff depletion. PUFFR, PUFFM, and DIFDEP are called from RATCHET.

Subroutine DIFDEP

Subroutine DIFDEP is the primary program element in the computation of diffusion, deposition, and depletion of the material in puffs. It implements the equations discussed in Sections 2.6 and 2.7. It also performs the transport computations for the puffs within advection periods.

DIFDEP is called once for each puff in each advection period. When DIFDEP is entered, the first function performed is the selection of the number of sampling intervals needed in the approximate integration of the concentrations and deposition at grid nodes. This determination is made on the basis of the ratio between puff movement during a sampling interval and the horizontal diffusion coefficient. The maximum number of intervals is established in the run-specification file. When the puff is small, the maximum number of sampling intervals may be used, but when the puff is large there is only one sampling interval. After the number of sampling intervals and the sampling interval duration have been selected, DIFDEP computes the distance traveled in each interval.

Having completed these preliminary steps, DIFDEP enters a computational loop that processes the puff. The code goes through the loop once for each sampling interval.

The order of operations in the loop is

- increment the puff age by the length of the sampling interval
- determine the surface roughness length and atmospheric conditions (stability, friction velocity, precipitation, etc.) at the position of the puff
- compute the diffusion coefficients, deposition velocity, and washout coefficient for the sampling interval
- compute the concentration at puff center, the vertical diffusion term, and ground-level concentration beneath the puff center
- compute time-integrated air concentrations and deposition at nodes near the puff
- adjust the mass in the puff to account for depletion resulting from deposition.

As the deposition and depletion calculations are made, the amounts of material being deposited and depleted are totaled for use in mass-balance calculations.

DIFDEP determines the diffusion coefficients for diffusion calculations using the approach described in Section 2.6.2 using functions PUFSIGY and PUFFSIGZ. The turbulence parameters used in computing the diffusion coefficients are estimated by functions TURBSIGV and TURBSIGW, which implement the equations presented in Section 2.6.3.

When the preliminary calculations are completed, DIFDEP determines the location of the puff and selects those computations that are appropriate for the location. If the puff is outside the model domain, the logical flag that indicates that the puff is active is set .FALSE., and the program returns to RATCHET. Otherwise, DIFDEP checks the concentration at ground level.

If the ground-level concentration beneath the center of the puff is greater than a threshold value, CHIMDT, DIFDEP continues with the accumulation of the time-integrated concentrations and deposition computations. Section 2.6.1 discusses the accumulation of the time-integrated air concentrations. Sections 2.7.2, 2.7.3, and 2.7.4 discuss the deposition calculation.

If the ground-level concentration is less than CHIMDT, DIFDEP jumps to the section that computes wet deposition, if there is precipitation. If there is no precipitation, DIFDEP returns to the main program.

When all diffusion and deposition computations for the sampling interval are complete, the mass in the puff is depleted to account for deposition and decay. Depletion of the puffs is discussed in Sections 2.7.5 and 2.7.6.

After depleting the puff, the pass through the sampling interval loop is complete. If there are more sampling intervals in the advection period, the process is repeated for the next interval.

Subroutine PUFFM

Subroutine PUFFM is used to determine the total puff movement during the advection period (60 min/NPH). The movement is computed in environmental grid units in four steps: 1) estimating the puff movement based on the winds at the puff's initial location, 2) using that movement to determine an approximate endpoint, 3) using the winds at the approximate endpoint and the initial position to estimate a second endpoint, and 4) averaging the two endpoint estimates.

If the puff transport height is above 10 meters, puff movement is computed using winds at the transport height. The transport-height wind is determined by first computing the 10-meter wind beneath the puff center and then adjusting the 10-meter wind using the diabatic profile implemented in the PROFILE function.

The method of estimating the wind beneath the puff center depends on the location of the puff. If the puff is within the computational domain (Cartesian grid), the wind is estimated from the four surrounding nodes using bilinear interpolation. If the puff center is on a boundary of the computational domain, the wind is determined by linear interpolation between two adjacent nodes. Finally, if the puff is outside of the computational domain, the wind at the closest node is used.

Subroutine PUFFR

Subroutine PUFFR assigns initial characteristics to each puff. When PUFFR is called, the first actions taken are to increment the total number of puffs, increment the number of puffs released from a specific source, and set the flag that indicates that the puff is active to .TRUE.

The puff location and transport height are then initialized. Two variables, QP and QPI, are used to track the mass in the puff. Both variables are given a mass equal to the product of the release rate and interval between puffs. The mass of the first variable, QP, remains constant as the puff moves through the model domain. The second mass is depleted as material in the puff deposits and decays.

Finally, each puff is assigned initial diffusion coefficients. The initial diffusion coefficients are set via the run-specification file. For simulations using four puffs per hour and a stack with a 20,000-cfm flow, initial diffusion coefficients of σ_z = 5.1 meters and σ_r = 10.3 meters give an initial concentration at the center of the puffs that is equal to the concentration in the stack.

4.3.4 Hourly and Daily Output Subroutines

The three subroutines discussed in this section provide the routine program output. Subroutine BALANCE writes a daily mass balance to the log file. Subroutine OUTPUT produces the primary output files for the program. When requested by the user, subroutine TESTM generates an hourly summary of puff positions for use in testing model performance.

Subroutine BALANCE

At the end of each day, subroutine BALANCE performs a series of calculations that provide checks on model arithmetic. The results of these checks are written to the log file. The individual elements of the mass balances are also written to the log file.

The first check is made on the airborne, undepleted mass. BALANCE computes the amount of material that should be in active puffs (QP) in the model domain at the end of the day by adding the mass released to the mass in the puffs active at the beginning of the day and subtracting the mass in the puffs that leave the domain. It also calculates the actual sum of the masses in the active puffs. These two sums, which should be identical, are written to the log file as the "NOBLE GAS" check.

The second check is made on the airborne, depleted mass. The mass in the active, depleted puffs (QPI) at the end of the day should be equal to the mass in depleted puffs at the beginning of the day plus the mass released during the day, minus the sum of the mass lost in transit by radioactive decay, the mass removed from the puffs to account for deposition, and the mass in the puffs leaving the domain. This sum is compared to the sum of the depleted mass in the puffs. These two sums are written to the log file as the "OTHER AIRBORNE" check.

The third check is made on the surface deposition. To perform the check, BALANCE computes the sum of the mass deposited minus the mass lost during the day by radioactive decay, and the sum over all nodes of the mass on the surface at the end of the day. These sums are written to the log file as the "SURFACE" check.

If the arithmetic in the code is correct, the numbers in each pair in the first three checks should be identical within the limits of computer round-off errors. The fourth check compares the mass deposited on the surface with the mass removed from the puffs. This is an approximate check. The difference between the numbers indicates the magnitude of the error associated with the assumption that mass per unit area on the surface at each node represents surface contamination for the area represented by each node on the concentration grid (36 square miles when the nodes are 6 miles apart).

The mass removed from a puff is based on an analytical integration of the deposition flux (e.g., $Ci/m^2\text{-}s^{-1}$) over the area covered by the puff and the time of deposition. The total mass removed is the sum over all puffs and time during the day. It should be exact within the limits of precision of the numbers used. In contrast, the amount deposited on the surface is an approximate value, estimated by multiplying deposition flux at the node by the area represented by the node and the time of deposition and then summing over the time and all nodes.

The "DEPOSITION/DEPLETION RATIO" is the ratio of the approximate amount of material deposited to the amount of material removed from puffs. The ratio should be near one. However, it can be as large as four or five and as small as 0.2 under unusual conditions. For example, ratios near 5 can be obtained if the release point is on a node and the wind direction is constant on a cardinal heading. In practice, the ratios tend to be between 0.5 and 2 when real meteorological data are used.

The individual mass-balance elements are written to the log file following the checks. The first four elements give the beginning mass, mass released, mass out, and remaining mass for the noble gas comparison. The next four elements give the same information for the other airborne comparison. The ninth element gives the mass on the surface at the end of the day. The next two elements give the mass lost by decay in the air and on the ground, respectively. Finally, the last four elements deal with deposition and depletion. The eleventh and twelfth elements give the approximate masses on the surface from low-level deposition processes (deposition velocity) and washout, respectively, and the last two elements give the mass removed from puffs by the two processes.

Subroutine OUTPUT

Subroutine OUTPUT writes the primary and secondary output files for the code. The primary output file contains the daily time-integrated air concentrations and surface contamination for the run segment. It is an unformatted binary file that is given the name entered in record 26 of the run-specification file. At the end of each simulated day, OUTPUT writes four records to the file. These are a daily heading for the time-integrated air concentrations, the time-integrated air concentration data (TICI), a daily heading for the surface-concentration data, and the surface-concentration data (SCI).

The secondary output file contains daily time-integrated air concentrations for a nondecaying, nondeposition tracer with the same release characteristics as the material of primary interest. This file is given the name entered in record 27 of the run-specification file. It is also an unformatted binary file. Two records are written to this file each day. They are a daily heading and the time-integrated air concentration (EXPCUM).

After writing the daily additions to the files, OUTPUT reinitializes the arrays used to accumulate the time-integrated air concentrations and surface contamination. It then returns control to the main program.

Subroutine TESTM

RATCHET calls subroutine TESTM at the end of each hour if the first character of the run title entered in the run-specification file is an asterisk (*). When called, the subroutine writes the date and time and the status of each puff to a test output file. The name of the test output file is created by RATCHET from the name of run-specification file by replacing the first two letters of the run-specification file name with the letters "ts".

The information written to the test output file includes the puff number and its source, the puff position on the wind grid (grid units) and its release height (m), the distance moved in the x and y directions in the last advection period (m), the diffusion coefficients at the end of the period (m), and undepleted and depleted activity or mass in the puff at the end of the period (Ci).

4.3.5 Housekeeping Subroutines

RATCHET contains two subroutines for housekeeping purposes called CLEAN2 and COMBINE.

Subroutine CLEAN2

Subroutine CLEAN2 is used to reduce the number of puffs that are being tracked by RATCHET. It is called at the end of each hour. Puffs are eliminated because they have been marked inactive.

Puffs are marked inactive by changing the value of MF( ) from one to zero. This change is made when a puff leaves the model domain. Puffs may also be marked inactive if the concentration at the center of the puff falls below the threshold concentration specified in the run-specification file.

Subroutine COMBINE

Subroutine COMBINE will be called at the end of each hour when puff consolidation is selected in the ninth record of the run-specification file. When called, the subroutine compares the ratio of the distance between the centers of consecutive puffs from the same source and the average diffusion coefficient of the puffs with the value of CLN_CRIT. If the ratio is less than CLN_CRIT, the puffs are combined because the information in the two puffs is not significantly greater than the information in a single puff. The position, diffusion coefficients, and age of the combined puff are mass-weighted averages of the values in the individual puffs.

The combined puff characteristics are assigned to the younger puff (higher number). The other puff is marked inactive by changing the value of MF( ) to zero. This puff will be deleted when CLEAN2 is called.

4.3.6 Segment-End Output Subroutines

The last subroutines used by RATCHET write the mass-balance summary and residual-puff data files at the end of each segment. The information in the mass-balance summary can be used to evaluate code performance or track the fate of effluents.

The information in the residual-puff data file may be used to initialize the model for a subsequent run segment.

Subroutine FBALANCE

Subroutine FBALANCE writes summary information on model performance to two files. It writes a complete summary to the log file and a limited summary to the mass-balance summary file named in record 29 of the run-specification file. The information written to the mass-balance summary file consists of the six items. These items are 1) the mass in the air in the domain at the beginning of the run segment, 2) the mass released during the segment, 3) the mass transported out of the domain during the segment, 4) the mass decaying in the air during transport within the domain, 5) the mass deposited by dry deposition of particles and wet and dry deposition of gases, and 6) the mass deposited by wet deposition of particles.

Subroutine PUFFOUT

Subroutine PUFFOUT creates the residual-puff data file at the end of each RATCHET simulation. It is called by the main program. The name for this residual-puff data file is entered in record 28 of the run-specification file. Note that the program will abort if this name duplicates an existing file name.

This file is opened as an unformatted, sequential file. PUFFOUT then writes the file name and status to the RATCHET log. If the file was opened successfully, the run title, run date, and run time are written to the file. This information is followed by the number of puffs on the grid at the end of the simulation and the information for each puff. The last items written to the file are the final seeds for use in random sampling. When the file is complete, PUFFOUT closes the file and notes the results on the log.

4.3.7 RATCHET Functions

The RATCHET code includes 19 functions. Three of the functions are used for time conversion. Fifteen functions provide information used in the transport, diffusion, and deposition calculations. The remaining function is the RATCHET random-number generator. This section briefly describes each of the functions. In general, the functions are short-code elements. They may include one or more branches, but the structure of the branches is simple.

Real Function DDEPVEL

Function DDEPVEL computes dry-deposition velocities. It implements Equations (2.51) through (2.53) for highly reactive gases, slightly reactive gases, and small particles.

Function input consists of friction velocity, 10-meter wind speed, effluent type, transfer resistances, and the fraction of the material in each partition. For noble gases (type = 0), DDEPVEL returns a deposition velocity of 0. For materials such as iodine (type = 4), DDEPVEL returns a weighted-average deposition velocity. The weights used in averaging are the partition fractions.

DDEPVEL assumes a minimum wind speed of 1 meter per second. If the wind speed passed to the function is less than 1 meter per second, the function uses a speed of 1 meter per second in computation of the aerodynamic resistance.

If the function encounters a type greater than 4, it will stop code execution.

Integer Function DTHOUR

In RATCHET, code actions, such as reading meteorological data and starting and stopping releases, are controlled by elapsed time in minutes from a predetermined reference. The reference time is specified in the run-specification file, which is read in subroutine SPECIN. However, meteorological and source-term data records include dates and times given in the form year, day of the year, and hour. Integer function DTHOUR converts these dates and times to elapsed time. The conversion takes leap years into account up to the year 2000.

All times are assumed to be standard times. The conversion process does not account for changes to and from daylight savings time.

Character Function HOURDT

Character function HOURDT converts the elapsed time used internally in RATCHET to an eight-character string that contains the day, month, year, and hour. The function is used in subroutines that write to output files to enable the program to provide dates and times in the familiar month/day/year hour:00 format.

The first two characters in the string returned by HOURDT are the last two digits of the year. The next two characters are the month (01 = January, etc.) The fifth and sixth characters are the day of the month, and the last two characters are the hour of the day. Hour of the day ranges from 00, for the hour beginning at midnight, to 23.

Real Function INVMOL

Function INVMOL converts a discrete atmospheric stability-class estimate into an estimate of the inverse of the Monin-Obukhov length (1/L). The inverse of the Monin-Obukhov length is used in scaling heights in the atmosphere and enters into calculation of u_*, wind profiles, mixing-layer depth and diffusion coefficients. The conversion is based on the relationship between surface roughness length, stability class, and 1/L shown in Figure 2.4.

The function is called with the following arguments: stability class, surface roughness length, lflg, and LSEED. Lflg is a logical flag used to control the selection of 1/L in the function. If lflg = .FALSE., the function will return a value for 1/L that is in the middle of the 1/L range, given the stability class and roughness length. If lflg = .TRUE., the function will select a value of 1/L at

random from a range calculated from the stability class and surface roughness assuming a uniform distribution of 1/L in the range. LSEED is the seed for the random-number generator.

Integer Function JULIAN

RATCHET requests dates for the beginning and end of the simulation and release. For convenience, these dates are requested in the standard month, day, year form. Integer function JULIAN takes this information and returns a day of the year ranging from 1 to 366. The conversion process accounts for leap years. These dates and times are converted to the elapsed time that RATCHET uses internally by function DTHOUR.

Real Function MIX_HT

Function MIX_HT is used to estimate the mixing-layer depth at meteorological stations. An estimate of the mixing-layer depth is calculated using Equations (2.10) or (2.11), as appropriate. This estimate is compared with a default value for the month and time of day, and a final value is selected using the rules set forth in Section 2.3.3. Input to MIX_HT consists of the friction velocity, the inverse of the Monin-Obukhov length, the stability class, the month, the hour, the array of default mixing depths, a random-number flag, and a random number between 0 and 1.

If mixing-layer depth random sampling has been selected, the random-number flag, Hlfg, will be .TRUE. When Hflg is .TRUE., the random number is used to calculate values for constants in Equations (2.10) and (2.11). Otherwise, the values shown in the equations will be used.

MIX_HT sets a stability index for use in determining the default mixing-layer depth based on the input stability class. The index ranges from 1 to 5. Stability classes 1 and 2 translate to an index of 1, stability classes 6 and 7 translate to an index of 5, and the remaining stability classes translate to an index of one less than the stability class number.

The stability indexes are checked for reasonableness based on time-of-day and season. If an unstable index is found at night, the index is changed to neutral. Similarly, if a stable index is found during the day in the summer, it is changed to neutral.

The rules used to select the mixing-layer depth are based on stability, time-of-day, and season. Stability classes are grouped into three categories—unstable, neutral, and stable. In selection of the mixing-layer depth, time-of-day is divided into day and night and the year is divided into two seasons. The division between day and night is based on the hours of sunrise and sunset at HMS (46°34'N, 119°36'W). These times, which are contained in DATA statements in the function, should be changed if MIX_HT is to be used for a location other than the HEDR atmospheric model domain. The two seasons used by the function are summer and winter. Summer is defined as April through September, and winter is the remainder of the year.

The range of mixing-layer depths is limited to 10 meters to 2000 meters. If the selection rules give a mixing-layer depth outside of this range, the appropriate upper or lower bound is returned as the mixing-layer depth.

Real Function MXLD_EST

Function MXLD_EST is used to compute the mixing-layer depths as they are needed in transport, diffusion, and depletion calculations. The input to the function consists of the x and y coordinates of the position in the environmental grid for the position for which the mixing-layer depth is needed and the coefficients for the plane used to represent the spatial variation of the mixing-layer depth.

The function uses the position and coefficients to calculate the mixing-layer depth. If the calculated depth is less than 10 meters, a mixing-layer depth of 10 meters is assumed. If the calculated depth is greater than 2000 meters, a depth of 2000 meters is assumed.

Real Function PLUMRISE

Function PLUMRISE implements Equations (2.12) through (2.23) described in Section 2.4.2. Input to the function consists of the stack height, radius and flow, effluent temperature, ambient air temperature, wind speed, stability class, and mixing-layer depth.

Two default conditions are included in the function code. If the stack height is greater than the mixing-layer depth, stability class 7 (extremely stable) is assumed for plume-rise calculations. Similarly, if the wind speed is less than 1.37 meters per second, the plume-rise calculations assume a speed of 1.37 meters per second.

Real Function PRCPRATE

Function PRCPRATE determines precipitation rates during periods of precipitation. The input to the PRCPRATE consists of the precipitation random-sampling flag, precipitation type and regime, precipitation rate cumulative frequency distributions, and a random number between 0 and 1. Default precipitation rates are included in a data statement in the function.

If the random sampling for precipitation rates is not selected, PRCPRATE will return the default rate for the precipitation type. Otherwise, PRCPRATE will use the random number, precipitation type, and precipitation regime to obtain a precipitation rate from the cumulative frequency distributions.

Precipitation rates returned by PRCPRATE are in millimeters per hour as required for use in the wet deposition calculations.

Real Function PROFILE

Function PROFILE implements Equations (2.8) and (2.9) described in Section 2.3.3. The input to the function is reference height for the known wind speed, known speed, surface roughness, friction velocity, reciprocal of the Monin-Obukhov length, stability class, and height for which the wind speed is desired. Figure 2.5 shows the increase in wind speed with height relative to the 10-meter wind speed for the seven stability classes.

Real Functions PUFSIGY and PUFFSIGZ

Functions PUFSIGY and PUFFSIGZ are used to calculate diffusion coefficients. PUFSIGY implements Equations (2.40) and (2.41) discussed in Section 2.6.2. PUFFSIGZ implements Equations (2.42) through (2.44), also discussed in Section 2.6.2.

The input for PUFSIGY consists of the horizontal turbulence component (σ_v), the proportionality constant (c_{sy}), the age of the puff, the duration of the time step, and the previous value of the horizontal diffusion coefficient. Input for PUFFSIGZ consists of the vertical turbulence component (σ_w), the stability class, the age of the puff, the duration of the time step, the puff-transport height, the mixing-layer depth, and the previous value of the vertical diffusion coefficient.

The growth of the horizontal diffusion coefficient is limited in all conditions to 100,000 meters. In contrast, the growth of the vertical diffusion coefficient is constrained by the depth of the mixing layer, which can change as a function of position. If the transport height is less than the mixing-layer depth, the vertical diffusion coefficient is limited to the depth of the mixing layer. If the transport height is greater than the mixing-layer depth, the vertical diffusion coefficient can only increase to the effective release height. However, in no case is a decrease in the mixing-layer depth permitted to cause a reduction in the vertical diffusion coefficient.

If the puff-transport height is greater than the mixing-layer depth, a slow increase in the vertical diffusion coefficient is assumed regardless of the stability class. The rate of growth assumed is the same rate used for stable atmospheric conditions.

Integer Function RAN_STAB

Function RAN_STAB is called in subroutine MET_FLD2 if random sampling of stability classes has been selected. Given the stability class reported for a meteorological station, it returns a random stability-class estimate for that station. The input to the function consists of the reported stability class, an array of conditional cumulative probability distributions from which the random samples are drawn, and a random number.

The array STABLE contains the conditional cumulative probability distributions. In the array, the distributions are associated with the first index and the reported stability is associated with the second index. For example, STABLE(I,4) contains the cumulative probability distribution from which the random sample is to be drawn when the reported stability is class 4.

Function RAN_STAB should work correctly with any pseudorandom-number generator that produces numbers in the range 0 to 1, regardless of whether the low end of the range is open or closed. Random values of less than 10^{-6} are assigned the value 10^{-6}, permitting zero to be used as a value in STABLE when zero is included in the range of the random-number generator. Without this precaution, there would be the remote possibility that a random number of zero could cause RAN_STAB to return a stability class of 1 regardless of the reported stability class.

Real Functions TURBSIGV and TURBSIGW

Functions TURBSIGV and TURBSIGW estimate the standard deviations of the horizontal and vertical components of the turbulence velocities, respectively. They implement Equations (2.45) through (2.50), which are discussed in Section 2.6.3.

The input to TURBSIGV consists of the stability class, friction velocity, puff transport height, mixing-layer depth, and reciprocal of the Monin-Obukhov length. Function TURBSIGW has the same input. In addition, input to TURBSIGW includes the horizontal turbulence velocity as the last argument.

Each function checks to ensure that the stability class is within the range 1 through 7. If it is not, code execution is stopped. If the stability class is within the range, the characteristic turbulence velocities are calculated by the appropriate equations for the stability.

The characteristic turbulence velocities, calculated by Equation (2.45) during stable conditions, go to 0 as the transport height approaches the top of the mixing layer and become negative when the transport height is above the mixing layer. To avoid any potential problems that this behavior might cause, Equation (2.45) is used only when the transport height is in the lower 90 percent of the mixing layer. When the transport height is in the upper 10 percent of or above the mixing layer, the characteristic turbulence velocities are calculated using Equation (2.46), which is Equation (2.45) evaluated at a transport height equal to 90 percent of the mixing-layer depth.

A value of σ_v calculated in TURBSIGV may be used as input to TURBSIGW. If the stability class is greater than 3 (neutral or stable) and σ_v is greater than 0, TURBSIGW will be set equal to σ_v and return to the calling subroutine. Otherwise, TURBSIGW will compute a value for σ_w using the appropriate equations.

Ultimately, TURBSIGV and TURBSIGW have a minimum value of 0.01 meters per second. If the calculated values are lower than 0.01 meters per second, a value of 0.01 meters per second is substituted for the calculated value.

Real Function U01

Function U01 is a congruential random-number generator. Press et al. (1986) and Kahaner et al. (1989) describe congruential random-number generators. Given a seed, which is entered via the agreement list, U01 returns a uniformly distributed pseudorandom number in the range 0 to 1 through the function name. In addition, the function returns a new seed via the argument list.

Real Function USTAR

Function USTAR calculates the friction velocity using the diabatic wind-speed profile equations, Equations (2.8) and (2.9). The input to the function includes the height at which the wind speed is known, the wind speed, the surface roughness length, the reciprocal of the Monin-Obukhov length, and the stability class.

The minimum friction velocity returned by the function is 0.01 meters per second. If a lower value is calculated, 0.01 meters per second is substituted for the lower value. A friction velocity of 0.01 meter per second is associated with wind speeds of less than 1 meter per second.

Real Function WDEPGAS

Function WDEPGAS calculates wet deposition velocities for slightly and highly reactive gases. It implements Equation (2.54) discussed in Section 2.7.3. Input to WDEPGAS consists of effluent type, fraction of effluent associated with each type, precipitation type and rate, ambient air temperature, and solubility coefficients.

WDEPGAS returns a value of 0 for the wet deposition velocity for type 0 (noble gas) and 3 (particulate) effluents. It will also return a value of 0 during snow when the temperature is less than -3.0°C. If the effluent type is 4, the function returns a weighted wet deposition velocity that accounts for wet deposition of both slightly and highly reactive gases.

WDEPGAS will stop code execution if it is called with a precipitation type that is less than 1 or greater than 6.

Real Function WDEPPART

Function WDEPPART calculates a washout coefficient for particles. It implements Equations (2.55) and (2.56) in Section 2.7.3. Input to WDEPPART consists of effluent type, fraction of effluent associated with each type, precipitation type and precipitation rate.

WDEPPART will return a washout coefficient of zero unless the effluent type is 3 (particle) or 4 (mixed). If the effluent type is 4, the washout coefficient returned by WDEPPART will be based on the fraction of the total effluent associated with particles. It will not include the wet deposition of any gases. Thus, if the mixture does not include any particles, the washout coefficient will be zero.

WDEPPART will stop code execution if called when the precipitation type is less than 1 or greater than 6.

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