NOAA Technical Memorandum ERL ARL-50

A REGIONAL-CONTINENTAL SCALE TRANSPORT, DIFFUSION, AND DEPOSITION MODEL

PART I: TRAJECTORY MODEL

Jerome L. Heffter
Albion D. Taylor

PART II: DIFFUSION-DEPOSITION MODELS

Jerome L. Heffter
Gilbert J. Ferber

Air Resources Laboratories
Silver Spring, Maryland
June 1975

UNITED STATES
DEPARTMENT OF COMMERCE
Rogers C.B. Morton, Secretary

NATIONAL OCEANIC AND
ATMOSPHERIC ADMINISTRATION
Robert M. White, Administrator

Environmental Research
Laboratories
Wilmot N. Hess, Director

CONTENTS

ABSTRACT

The Air Resources Laboratories has developed a computerized post-facto trajectory model intended primarily for calculating the transport, diffusion, and deposition of effluents on regional and continental scales. A month, season, or year of trajectories at 6-hourly time intervals may be calculated forward or backward in time from any origin in the Northern Hemisphere for durations up to 10 days. Trajectory computations use winds at any altitude above sea level or winds averaged through any desired layer above average terrain. Computer output includes a listing of individual trajectory end points after selected durations, plotted trajectories for any desired map scale on either Mercator or Polar Stereographic projections, and plotted maps showing percent frequency of trajectory traverses over grid squares.

A Gaussian plume model is combined with the trajectory model to calculate long-term (monthly, seasonal, annual) mean ground-level air concentrations and deposition amounts. Both wet and dry deposition are incorporated in the model. Another model calculates short-term (once or twice a day) mean ground-level air concentrations for selected sampling stations. Computer output includes plotted maps showing long-term concentrations and deposition amounts, and tables of short-term concentrations where the contributions from individual plumes are identified.

A REGIONAL-CONTINENTAL SCALE
TRANSPORT, DIFFUSION, AND DEPOSITION MODEL

PART I

TRAJECTORY MODEL

Jerome L. Heffter
Albion D. Taylor

1. INTRODUCTION

The Air Resources Laboratories (ARL) has developed a computerized post-facto trajectory model intended primarily for use in calculating the transport, diffusion, and deposition of effluents on regional and continental scales. The trajectory transport section of the model is described here; the diffusion and deposition sections are described in Part II.

The computer model was designed to efficiently calculate the large numbers of trajectories needed to evaluate specific pollution problems and also to be used as a research tool to investigate long-range transport and diffusion mechanisms. A continuing program of research and field experiments is in progress to verify and improve the model.

In its present form, a month, season, or year of trajectories may be calculated (1) from any origin in the Northern Hemisphere, (2) at 6-hour time intervals, (3) from one to ten days in duration, and (4) forward or backward in time.

Trajectory computations use winds at any desired altitude above sea level or winds averaged through any desired layer above average terrain, up to about 5 km. The wind input is obtained from observed winds at reporting pibal and rawinsonde stations or analyzed wind fields at grid points.

The types of output now available are:

1. Tables giving details of trajectory computations.
2. A listing or punched data cards giving trajectory end points at selected durations.
3. Trajectories plotted on any desired map scale for either Mercator or Polar Stereographic projections.
4. Maps showing percent frequency of trajectory traverses over grid squares during a month, season, or year.
5. Trajectory and wind-rose percent frequencies by sector.
6. Maps showing long-term average surface air concentrations.

7. Maps showing long-term average surface air concentrations depleted by dry and wet deposition and maps of surface deposition amounts.

8. Short-term average surface air concentrations at a point (or several points) including a tabulation of the plumes that contributed to each concentration and the amount contributed.

Items 1 through 5 are described here and items 6 through 8 are discussed in Part II.

2. INPUT DATA

The user has the option to select as input either observed winds, analyzed winds, or both. Observed winds are recommended as the basic input. However, in areas of sparse wind observations, such as over the oceans, analyzed winds should be used. The use of both types of wind input is often desirable where trajectories are expected to traverse land and ocean areas.

2.1 Observed Winds

The observed winds used in the model are available on magnetic tapes (USAF-ETAC). These tapes constitute a unique set of meteorological data organized by time sequence: worldwide and upper air reports for all reporting stations are grouped together for each observation time. Information for each reporting station includes station identification (WMO block-station number), location (latitude, longitude), and elevation (meters above sea level), as well as time of observation (00Z, 06Z, 12Z, 18Z) followed by two data groups. The first group contains the upper air wind data and the second contains upper air temperature and humidity data. One month of information organized by time for all stations in the Northern Hemisphere is packed onto three magnetic tapes (seven-track, 800 bits per inch); the first contains days 1 through 10; the second contains days 11 through 20; the third contains the remaining days in the month.

The data in the first group include wind speed (m/sec), wind direction (degrees), height (m), and pressure (mb). For use in the model, data are extracted to provide coverage for a particular area of interest (e.g., 48 states and southern Canada) for all heights up to about 5 km. These data are unpacked and written on an "operational" series of tapes. Each tape in this series contains about three or four months of wind data, which can be used as input to trajectory computations for a season or a year without a great deal of tape manipulation. The data in the second group (temperature, humidity) are not presently being used in the model.

2.2 Analyzed Winds

Analyzed meteorological information, also available on magnetic tapes (NOAA-NWS, 1972), is in the form of two data analyses per day (00Z and 12Z) at each grid point of the Northern Hemisphere octagonal grid (1966 points) for standard pressure levels (1000, 800, 700, 500 mb, etc.). One month of analyses is packed on two magnetic tapes (seven-track, 800 bits per inch); the first contains days 1 through 15; the second contains the remaining days in the month.

Wind information is available as u and v components (m/sec) at each of the 1966 grid points (NOAA-NWS, 1971). For use in the model the wind components at each grid point at 1000, 800, 700, and 500 mb are unpacked and written on an "operational" series of tapes. Each tape contains about three or four months of wind data.

2.3 Average Terrain

The terrain heights used in the model are obtained from data tapes giving terrain height averages in one-degree squares over the world (Smith et al., 1966).

3. TRANSPORT MODEL

3.1 Observed Wind Input

A trajectory is composed of a series of 3-hour segments. Each segment is computed assuming persistence of the winds reported closest to the segment time. For example, for a 3-hour segment from 00Z to 03Z we assume 3-hour persistence of the 00Z winds; the 3-hour segment continuing from 03Z to 06Z is computed assuming 3-hour backward persistence of the 06Z winds; and for the segment from 06Z to 09Z we assume 3-hour persistence of the 06Z winds, etc.

The observed winds used in the computations are either those at a desired trajectory level or those averaged throughout a desired layer above the average terrain height. In practice, we assume that, over regional-to-continental distances, an effluent released in the boundary layer (surface to about 2000 m) is transported by the average wind in the afternoon mixing layer. Seasonal values for the top of the afternoon mixing layer have been determined in the contiguous U.S. (Holzworth, 1972). The base of the transport layer is usually assumed to be 300 m above average terrain to eliminate surface frictional effects that tend to slow down average transport speeds.

The average wind in a layer is computed from the reported winds linearly weighted according to height (see fig. 1).

$$V_i = \frac{\sum^{\text{layer}} H_l \, V_l}{\sum^{\text{layer}} H_l} \qquad (1)$$

where V_i is the average wind in the layer at station i, V_l is a reported wind at level l, and H_l is a linear height weighting factor.

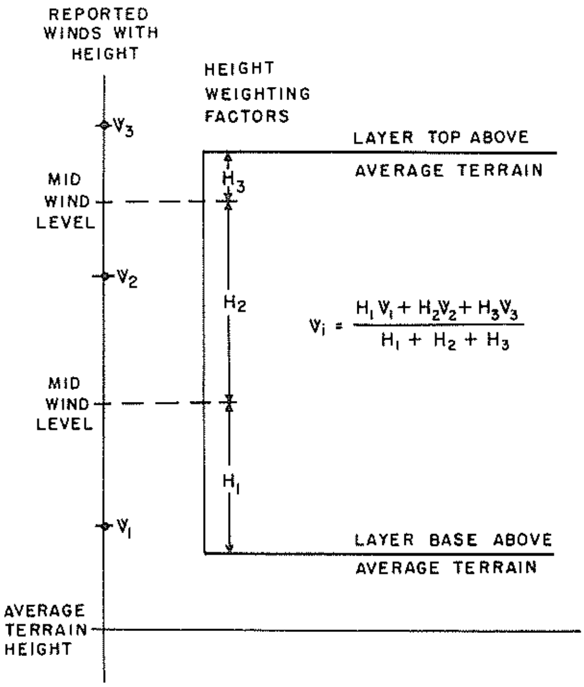

Figure 1. Scheme for determining an average wind in a layer.

Each trajectory segment computed from observed winds is given by (see fig. 2):

$$TS_O = \frac{\sum^{R} DW_i \; AW_i \; TS_i}{\sum^{R} DW_i \; AW_i} \tag{2}$$

where TS_O is the trajectory segment computed from observed winds;

$\sum^{R}$ indicates the summation over all observed winds within a radius R of the segment origin;

$TS_i = (V_i)\ (\Delta t)$, is the contribution to the trajectory segment from an observed wind V_i and Δt is the segment time interval;

$DW_i = f(dw_i)$, is the distance weighting factor, a function of dw_i, the distance from an observed wind to the mid-point of TS_i; and

$AW_i = f(\theta_i)$, is the alignment weighting factor, a function of θ_i, the angle formed between TS_i and a line drawn from the segment origin to a wind observation point.

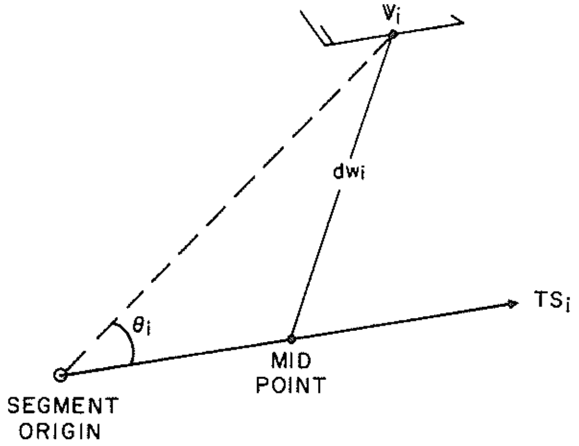

Figure 2. Configuration for determining a trajectory segment from observed winds.

The user may select various parameter values to be used in the model. He may also select criteria that must be met in order to compute trajectory segments. If the criteria are not met, the trajectory is terminated.

The following are parameter values (Heffter, 1973) currently used in the model.

1. Time interval: $\Delta t = 3$ hours.
2. Radius: $R = 300$ nautical miles.
3. Distance weighting factor: $DW_i = 1/dw_i^2$(the closest observations receive the greatest weight).
4. Alignment weighting factor: $AW_i = 1\text{-}0.5|\sin\theta_i|$ (observations upwind and downwind receive the greatest weight).

The current criteria for reported wind input data needed to compute a trajectory segment are as follows:

1. At least two reporting wind levels at a reporting station for averaging in the chosen layer.
2. At least two reporting station locations within radius R or one station located within 0.5R.

3.2 Analyzed Wind Input

The grid winds used in the computations either are taken at the desired level or are averaged throughout any desired layer above the average terrain height. The average wind (V_i) in a layer at a grid point is determined the same as an average observed wind in a layer.

Each trajectory segment is computed using a wind at the segment origin as determined from bilinear interpolation between analyzed winds at the four corners of the grid square containing the segment origin. Computations are made assuming (see fig. 3):

$$TS_A = V\ (\Delta t); \qquad (3)$$

where TS_A is the trajectory segment computed from analyzed winds, Δt is the time interval, and V is the computed wind at the segment origin. We obtain V from:

$$V = (V_T - V_B)\ (Y/L) + V_B;$$

where $V_B = (V_2 - V_1)\ (X/L) + V_1$ and $\qquad (4)$

$$V_T = (V_4 - V_3)\ (X/L) + V_3.$$

L is the grid square length, V_1, V_2, V_3, and V_4 are the analyzed winds at the corners of the grid square, and X and Y are the component distances from the grid square corner to the segment origin.

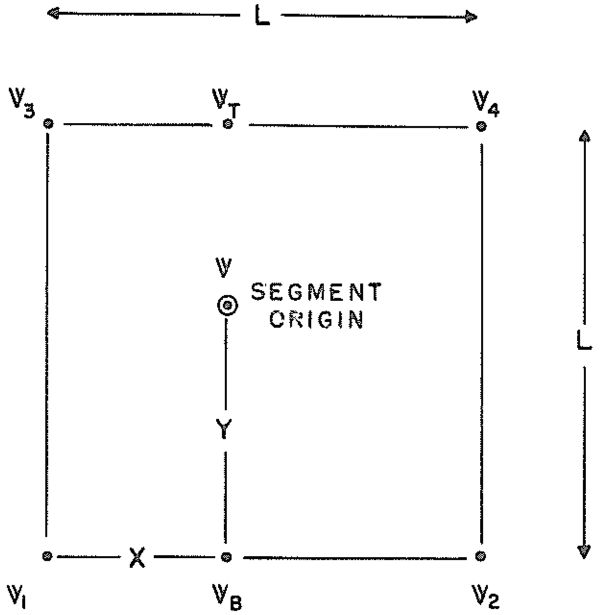

Figure 3. Configuration for determining a trajectory segment from analyzed winds on a grid.

3.3 Trajectory Calculations

Trajectory segments are linked together to produce a complete trajectory. Specifically, the first segment starts from the source and each following segment starts from the end point of the segment before it. Trajectories terminate after the desired duration or when the specified criteria are not met.

Trajectories are usually started from a source four times daily, 00Z, 06Z, 12Z, and 18Z. The model can start trajectories twice a day or eight times a day.

Trajectory durations are currently restricted to 10 days because of computing time and capacity limitations. Remember that great care should be taken in interpreting individual trajectories longer than 3 to 4 days duration. The value of long duration trajectories is probably greatest when they are considered in a climatological sense. To develop a trajectory climatology, we must use input wind data for times other than those closest to segment time. The reason for this is that many trajectories are terminated prematurely because the criteria for input wind data closest to segment time are not met. This results in too few long duration trajectories being completed. Therefore, a hierarchy of acceptable input data has been established.

When only 6-hourly observed winds are used as input, the hierarchy of acceptable input winds for calculating a trajectory segment is as follows:

1. Observed winds closest in time: 0 to 3-hour persistence.
2. Observed winds 2nd closest in time: 3 to 6-hour persistence.
3. Observed winds 3rd closest in time: 6 to 9-hour persistence.
4. Trajectory calculation terminated.

An example follows. When the observed 12Z input wind criteria are not met, the 3-hour 09Z to 12Z segment is computed using 3 to 6 hour persistence of the 06Z winds. If the 06Z input wind criteria is not met, the same segment is computed using 6 to 9 hour backward persistence of the 18Z winds. If the 18Z input wind criteria is not met, the trajectory calculation is terminated.

For 12-hourly analyzed winds alone the hierarchy is:

1. Analyzed winds closest in time: 0 to 6-hour persistence.
2. Analyzed winds 2nd closest in time: 6 to 12-hour persistence.
3. Trajectory calculation terminated.

When both observed and analyzed winds are used as input the hierarchy is:

1. Observed winds closest in time: 0 to 3-hour persistence.
2. Analyzed winds closest in time: 0 to 3-hour persistence.
3. Observed winds 2nd closest in time: 3 to 6-hour persistence.
4. Analyzed winds 2nd closest in time: 3 to 6-hour persistence.
5. Trajectory calculation terminated.

3.4 Trajectory Statistics

The computed trajectories are computer oriented on a gridded map, with preselected grid spacings, over the desired areal coverage. A count is kept as each grid box is traversed by a trajectory segment. The process is continued for the entire trajectory. If the same trajectory traverses a grid box more than once, the count is still taken as one traverse. The traverses for all of the trajectories are then accumulated in each grid box and divided by the total number of trajectories considered which gives a map of the percentage of trajectory traverses.

4. INPUT PARAMETERS

The input to each computer run includes the following data cards:

1. The origin of the trajectories (three letter identification, latitude, and longitude).
2. The date trajectory computations begin and the number of days for which trajectory computations are desired (should not exceed the number of days of wind input data on card 4).
3. Forward or backward in time for trajectory computations ("FORW" for forward or "BACK" for backward) and the number of days duration for the trajectories.
4. The number of days of wind input data (should be at least one day more than the trajectory duration on card 3).
5. The type of wind input data ("OBS" for observed winds only, "ANA" for analyzed winds only, or "O,A" for both types of wind input).
6. The geographical boundaries within which observed winds are considered for trajectory calculations (top and bottom latitudes; left and right longitudes).
7. The grid boundaries within which analyzed winds are considered for trajectory calculations (top and bottom grid row; left and right grid column).
8. The transport layer base and top, in meters above average terrain, in which the winds are to be averaged.
9. The geographical boundaries for maps in the plotting subroutines.

5. OUTPUT PARAMETERS

The amount and type of computer output can be designated by the user. Some output is designed to give the user specific detail on input data and trajectory calculations. Other input shows the calculated trajectory positions in tables. Still other output, called by subroutine, shows the trajectories on maps. Also available on maps are climatological trajectory summaries and long-term concentration and deposition information. Short-term concentration information is given in tables. Finally, a trajectory versus wind-rose comparison subroutine is available.

5.1 Computer Run Identification

Each computer run is identified by printing out all information on the input data cards. In addition, date-time identification is read from the input wind tapes and printed out to ensure that the proper input wind information is being used.

5.2 Tabulated Computational Details

There are three output features in the model that give details of trajectory segment computations: the first two are optional and the third is printed as part of each operational computer run.

1. The calculated average winds for all stations at any chosen time may be printed. Each row in the listing gives the WMO block station number, station height (meters MSL), average terrain height (meters MSL), the transport layer base and top height (meters MSL) above average terrain at the station, the number of reported winds at levels used to compute the average layer wind, and the average layer wind (direction in degrees and speed in meters per second). Also given are the individual reported winds used in the averaging calculation.

2. The calculated average wind at each station within the specified radius for every trajectory segment calculation may be printed for the trajectories at any time the user chooses. Each row in this listing gives the trajectory identified by date-time, a trajectory segment identifier, the calculated average wind (in component form) for the segment displacement, the location of each wind reporting station within the specified radius (in component form with respect to the segment), and the calculated average wind at each station (in component form). This information can be readily hand plotted on graph paper if detailed information about the displacement of any one or several segments is desired.

3. A table is printed giving the number of reporting stations within a specified radius, followed by a symbol for the time of the input winds, for each trajectory segment displacement calculation (see table 1). This table, programmed as part of each operational run, is valuable as a quick indicator of trajectory reliability. The symbols used in this table are:

For 6-hourly observed winds alone:

1. No symbol for observed winds closest in time.

2. "+" for observed winds 2nd closest in time.

3. "-" for observed winds 3rd closest in time.

For 12-hourly analyzed winds alone:

1. "." for analyzed winds closest in time.

2. "*" for analyzed winds 2nd closest in time.

For both observed and analyzed winds:

1. No symbol for observed winds closest in time.

2. "." for analyzed winds closest in time.

3. "+" for observed winds 2nd closest in time.

4. "*" for analyzed winds 2nd closest in time.

		3-HOUR SEGMENTS															
START DATE	START TIME	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
22	00Z	4	3	2	3	3	2-	2+	2	2	2+	2-	2	2	2+	3-	3
22	06Z	3	6	5	4	3	5	4	3+	3+	5	4	3+	3+	3	3	3+
22	12Z	5	7	5	6	6	5	6	7	6	7	7	7	6	4	5	5
22	18Z	6	6	6	6+	6+	5	3	2	2	2	3	4+	2+	2	2	2+

Table 1. The number of reporting stations and code for the time of the input winds for each 3-hour trajectory segment displacement calculation. (The code is described in the text.)

We will illustrate this with the example shown in table 1. If the number of reporting stations for each segment of a trajectory is greater than 4 or 5 (table 1; day 22-12Z) sufficient wind information was available for a more reliable trajectory than the one with many "+" and "-" symbols (table 1; day 22-00Z).

5.3 Tabulated Trajectory Positions

The latitude and longitude of trajectory segment endpoints at duration intervals chosen by the user are printed or punched on cards for each trajectory as part of each operational run (see table 2). A trajectory that was terminated for not satisfying operational criteria is identified by a latitude ≥ 99 and longitude ≥ 999.

```
                                  DURATION (HOURS)
                   12              24               36              48
  START
DATE TIME
  17   00Z   43.1 109.0    43.0 106.4    42.8 103.2    42.0 100.2

  17   06Z   42.8 110.1    42.6 107.5    99.8 999.8    99.8 999.8

  17   12Z   42.6 111.3    41.9 108.2    40.0 104.7    37.0 102.9

  17   18Z   42.9 111.2    41.7 106.9    39.3 103.7    35.6 102.8
```

Table 2. The latitude and longitude of trajectory segment endpoints at 12-hour intervals.

5.4 Subroutines

Model subroutines plot information on maps of computer page size (11 inches x 15 inches), eight lines to the inch. Either Mercator or Polar Stereographic projections are available. Map scales can be chosen by the user.

1. The individual trajectory plotting subroutine plots up to four trajectories per day on each computer page (see fig. 4).* Trajectories are coded A, B,C, and D for starting times at 00Z, 06Z, 12Z, and 18Z, respectively. Coded trajectory durations 1, 2, 3, ... for 6, 12, 18, ... hours, respectively, replace the coded letters at 6-hour intervals along each trajectory. All codes are printed as part of this subroutine.

2. A subroutine is available that plots a map showing the frequency (in percent) of trajectory traverses during any desired period: a week, month, season, or year (see fig. 5). For any operational run, a separate percentage frequency map for trajectories of various specified durations can be plotted. Included at the top of each map is the total number of trajectories used in the computations.

3. Another subroutine is available for comparing wind-rose and trajectory percent frequencies in sixteen 22.5 degree sectors around an origin for any desired period (e.g., a month, season, or year). A map of trajectory percent frequencies by sector out to a selected radial distance and by up to 20 radial distance intervals is computer plotted (see fig. 6). The wind rose statistics are based on average winds used for the first segment of each trajectory, and these statistics are hand-plotted in circles for ease of comparison with the hand-analyzed trajectory statistics.

---

*Political boundaries and isopleths in the figures are hand drawn.

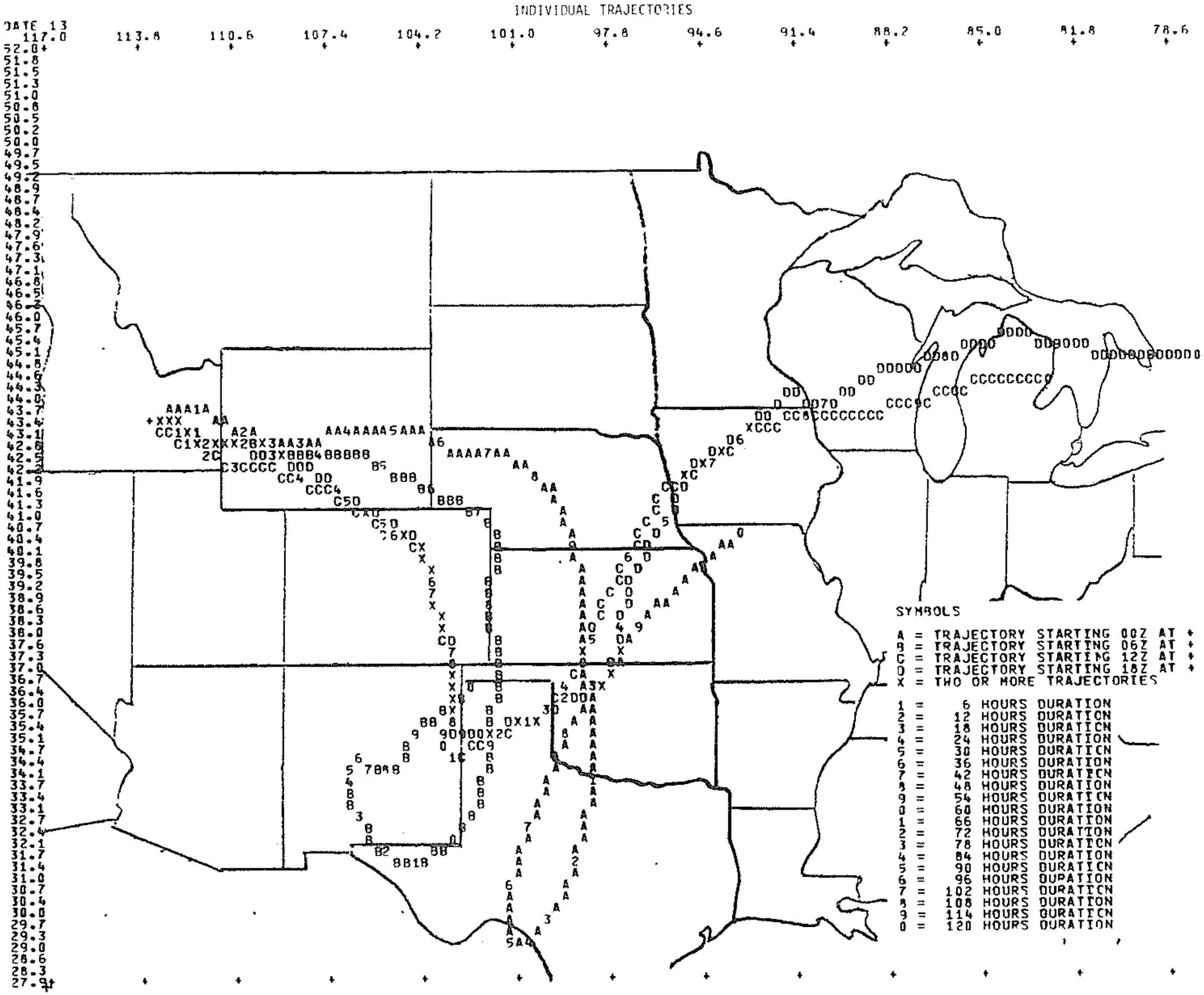

Figure 4. Individual trajectories.

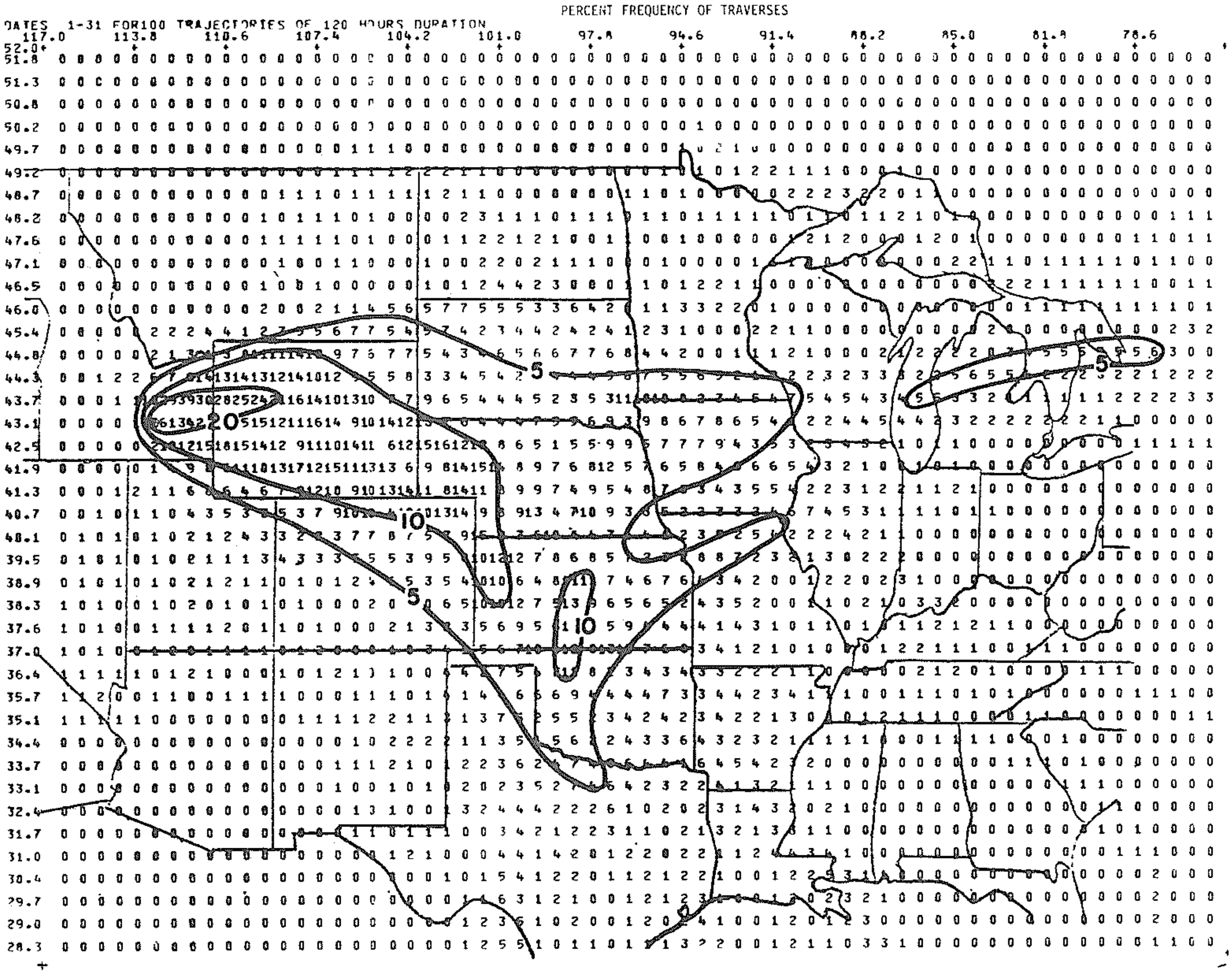

Figure 5. Percent frequency of trajectory traverses.

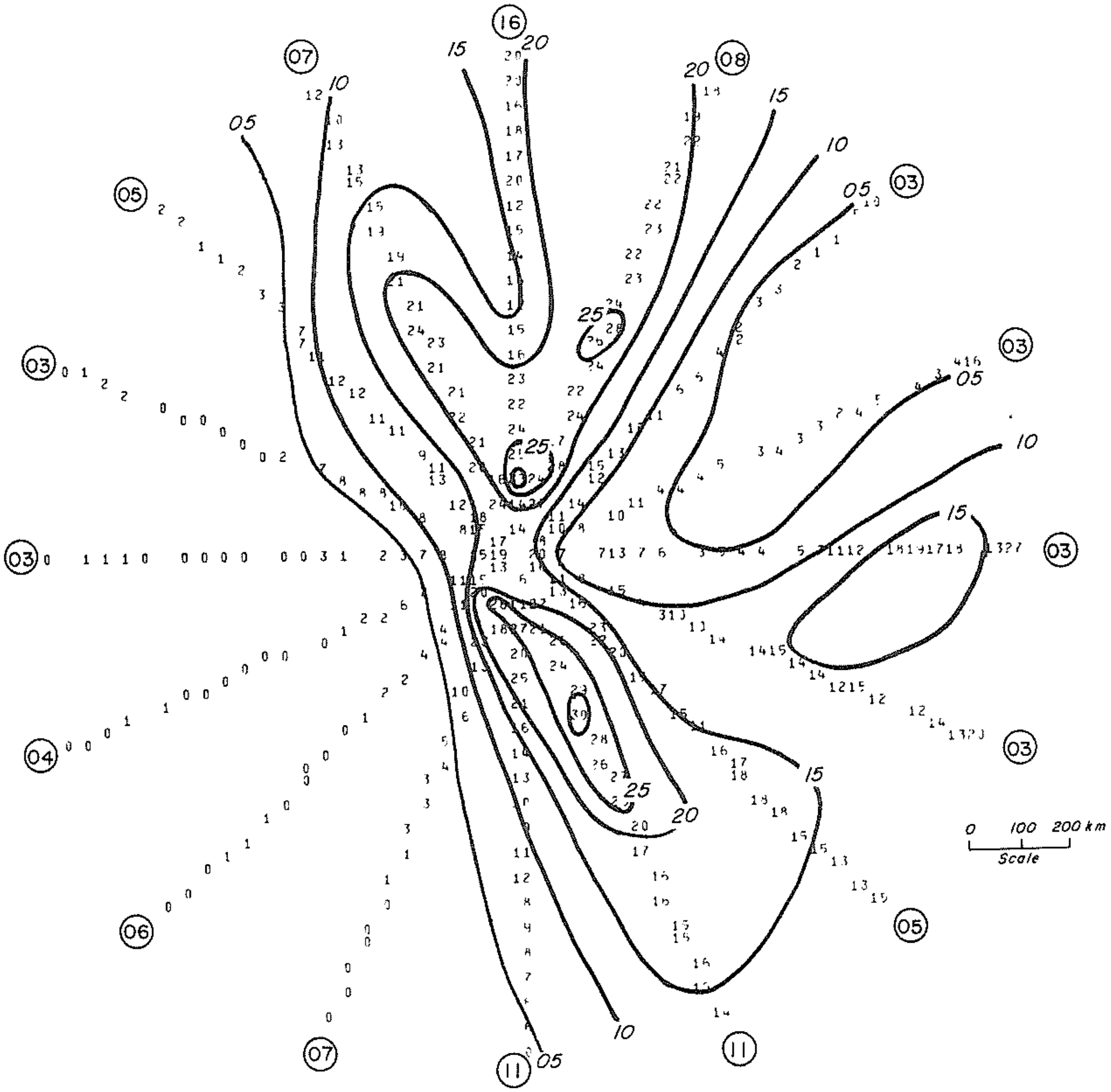

Figure 6. Wind-rose (circled) and trajectory percentage frequencies by sector.

6. ACKNOWLEDGEMENTS

The authors would like to thank the USAF - Environmental Technical Applications Center for supplying us with tapes of upper air meteorological data, and especially Sgt. D. Baily whose efforts made the inter-agency cooperation so successful.

This work was supported by the USAF - Technical Applications Center and the Division of Biomedical and Environmental Research, Energy Research and Development Administration.

7. REFERENCES

Part I

Heffter, J.L., 1973: "Trajectory Programs," in Atmospheric Transport and Dispersion of Pollutants and Related Meteorological Studies, July 1971-June 1972 (Robert J. List, Editor), NOAA Technical Memorandum ERL ARL-40, National Oceanic and Atmospheric Administration, Environmental Research Laboratories, Air Resources Laboratories, Silver Spring, Md.,pp. 21-45.

Holzworth, G.C., 1972: "Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution Throughout the Contiguous United States," Environmental Protection Agency, Office of Air Programs, Pub. No. AP-101, Research Triangle Park, North Carolina, pp. 32-35.

National Oceanic and Atmospheric Administration - National Weather Service (NOAA-NWS), 1971: "New Initialization Procedure for the C-layer (PE) Numerical Procedure Model," Weather Analysis and Prediction Division, Camp Spring, Maryland.

National Oceanic and Atmospheric Administration - National Weather Service (NOAA-NWS), 1972: "GRDARK Upper-Air Meteorological Data," Analysis Branch, World Weather Building, Camp Springs, Maryland.

Smith, S.M., Menard, H.W., and Sharmin, G., 1966: "World Wide Ocean Depth and Land Elevations Averaged for One Degree Squares of Latitude and Longitude," Scripps Institute of Oceanography, La Jolla, Calif. (Available from National Oceanic Data Center, Navy Yard Annex, Washington, D.C.).

United States Air Force - Environmental Technical Applications Center (USAF-ETAC), 1972: "DATSAV-SYNFILE Upper-Air Meteorological Data," Washington Navy Yard Annex, Washington, D.C.

PART II

DIFFUSION-DEPOSITION MODELS

Jerome L. Heffter
Gilbert J. Ferber

1. INTRODUCTION

The Air Resources Laboratories is developing a global model (Machta et al., 1974) for computing long-term air concentrations and resulting population exposures from pollutants released into the atmosphere. The model considers the fate of gaseous or particulate emissions from a uniform, continuous point source; treating local, regional, continental, and global scale dispersion in successive phases. The trajectory model described in Part I, combined with a Gaussian plume model, is the basis for calculations out to several thousand kilometers from a source. The model produces maps of mean monthly, seasonal, or annual air concentrations, deposition amounts, and population exposures. It is intended for use where long-range plume effects are important. The current version does not provide detailed calculations in the immediate vicinity of the pollutant source. The model includes deposition by wet and dry removal processes. Resuspension of deposited material is not considered, but this feature could readily be incorporated.

Another model (see sec. 3) uses the trajectory program to calculate short-term average air concentrations (e.g., 12-hr or 24-hr) at specified locations. Short-term source strength fluctuations are incorporated in this model so that short-term concentrations can be more precisely calculated. This is particularly useful for model verification where calculated concentrations from a known source, for specified sampling periods, can be tested against observed sample concentrations.

2. DIFFUSION-DEPOSITION MODEL FOR LONG-TERM CONCENTRATIONS

Trajectories are started from a source point four times per day and diffusion-deposition calculations are made along each trajectory. Mean ground-level air concentrations and deposition amounts are accumulated at grid points covering a selected area for any desired time interval (for example, a month, season or year).

2.1 Calculation of Air Concentration

Ground-level air concentration calculations along a trajectory are based on the Gaussian plume equation (Turner, 1970) for a continuous point source, also assumed to be at ground level

$$X_g = \frac{Q}{\pi \sigma_y \sigma_z \bar{u}} \exp(-y^2/2\sigma_y^2) \qquad (1)$$

where χ_g = ground-level air concentration (e.g., Ci/m^3)

Q = emission rate (Ci/sec)

σ_y = crosswind standard deviation of the plume (m)

σ_z = vertical standard deviation of the plume (m)

$\overline{u}$ = mean wind speed affecting the plume (m/sec)

y = crosswind distance from trajectory segment (m).

The vertical diffusion coefficient, K_z, may be substituted for σ_z, assuming

$$\sigma_z = (2K_z t)^{1/2} \qquad (2)$$

where t is the plume travel time (sec). Thus, ground-level air concentrations are calculated by

$$\chi g = \frac{Q}{\pi \sigma_y (2K_z t)^{1/2} \overline{u}} \exp(-y^2/2 \sigma_y^2) . \qquad (3)$$

The value of K_z may be specified by the user; at present we are using K_z = $5m^2/sec$ as an average value for the lower troposphere.

In some applications it may be preferable to assume that the effluent is uniformly dispersed through some specified mixing layer rather than assuming a Gaussian distribution in the vertical. If this option is chosen, surface air concentrations are calculated by

$$\chi g = \frac{Q}{(2\pi)^{1/2} \sigma_y L \overline{u}} \exp(-y^2/2 \sigma_y^2) \qquad (4)$$

where L, the depth of the mixing layer (m), is an input parameter to be specified by the user.

The model currently uses the approximation that

$$\sigma_y \text{ (meters)} = 0.5t \qquad (5)$$

where t is travel time (sec). This appears to be a reasonable approximation for several days travel time based on a variety of diffusion data summarized by Heffter (1965).

This model is designed primarily for calculations from about 100 km to a few thousand km from a source. The user is cautioned that several simplifications, incorporated to reduce computing time, might be undesirable for calculations in the immediate vicinity of a source. For example, stack height can be an important factor in determining air concentrations near a source, but it is not incorporated in Eq. (3) or (4). A more detailed treatment of both horizontal and vertical diffusion as a function of atmospheric stability also would be desirable in this region. Work is in progress to develop a more sophisticated trajectory-cum-dispersion model for the region within about 100 km of a source. It is expected that a trajectory model will prove superior to present techniques using stability-wind rose data.

2.2 Calculation of Dry and Wet Deposition

The concept of deposition velocity is used to calculate dry deposition amounts along a trajectory assuming

$$D_d = X_g \; V_d \; (\Delta t) \qquad (6)$$

where D_d is the amount deposited per unit area during the interval, Δt; X_g is the ground-level air concentration; V_d is the deposition velocity; and Δt is the time interval represented by each trajectory (e.g., 6 hours if trajectories are started four times per day).

Deposition velocity is dependent on particle size, wind speed, surface roughness, and other parameters. Most experimentally determined values are in the range from about 0.1 to a few cm/sec. The user must specify an appropriate value for his particular problem.

Precipitation scavenging is a second mechanism for plume depletion and ground deposition. Model calculation of wet deposition is based on an empirically derived average scavenging ratio (Engelmann, 1970) $E = X_w/\overline{X}_a$, where X_w is the concentration in rainwater at the ground and $\overline{X}_a$ is the mean concentration in the column of air from the ground to the top of the rain bearing layer. Wet deposition at a grid point along a trajectory is then

$$D_w = \overline{X}_a \; EP \; (\Delta t) \qquad (7)$$

where D_w is wet deposition per unit area during the time interval, Δt, and P is the precipitation rate.

With a Gaussian distribution in the vertical, the mean concentration in the column, $\overline{X}_a$, is readily obtained from the calculated ground concentration, X_g. The concentration integral, I, through the column is

$$I = X_g \int_0^\infty \exp\left(-z^2/4\, K_z t\right) dz. \qquad (8)$$

Integrating

$$I = X_g \; (\pi K_z t)^{1/2} \qquad (9)$$

and assuming that the plume does not extend above the rain layer, Δz, the mean concentration in the layer is simply

$$\overline{X}_a = I \; (\Delta z)^{-1} = X_g \; (\pi K_z t)^{1/2} \; (\Delta z)^{-1}. \qquad (10)$$

Substituting for $\overline{\chi}_a$ in Eq. (7), we obtain

$$D_W = E \; P \; \chi_g \; (\pi K_z t)^{1/2} \; (\Delta z)^{-1} \; (\Delta t) \qquad (11)$$

for deposition by precipitation scavenging.

The choice of an appropriate value for E is difficult since the scavenging ratio varies by more than a factor of ten, depending on rainfall rate, atmospheric stability, particle characteristics, and other variables, some of which have not yet been thoroughly explored. A value of 500 (mass ratio) was chosen as a reasonable average since it is about in the middle of the range of measured values. This is equivalent to a ratio of 4.2×10^5 by volume, which is currently used in the model. The user may substitute any other value he thinks appropriate.

2.3 Combined Diffusion-Deposition

The effects of wet and dry deposition are incorporated in the diffusion model as source depletion terms. The fraction of the source remaining airborne along a trajectory can be determined by integrating both wet and dry deposition over time. Since horizontal diffusion does not affect the rate of deposition, the effective source depletion is equal to the depletion of the column integral, I in Eq. (9). The depletion of the column integral with time is equal to dry removal plus wet removal; or from Eqs. (6) and (11),

$$\frac{dI}{dt} = -\chi_g \; (V_d + EP \; (\pi K_z t)^{1/2} \; (\Delta z)^{-1}). \qquad (12)$$

If we combine Eqs. (9) and (12) and rearrange terms,

$$dI/I = -(V_d \; (\pi K_z t)^{-1/2} + EP \; (\Delta z)^{-1}) \; dt. \qquad (13)$$

Integrating from t_o to t, we obtain

$$\ln(I_t/I_o) = - \left[(2 \; V_d \; t^{1/2})(\pi K_z)^{-1/2} + EPt \; (\Delta z)^{-1}\right] \qquad (14)$$

or

$$I_t = I_o \; \exp - \left[2 \; V_d \; t^{1/2} \; (\pi K_z)^{-1/2} + EPt \; (\Delta z)^{-1}\right] . \qquad (15)$$

The exponential term in Eq. (15) can be used as a factor applied to the emission rate, Q, in Eq. (3) to obtain an effective depleted source-term to account for dry and wet deposition. Thus the complete expression used to calculate surface air concentration is

$$\chi_g = \frac{Q \; \exp\left[- \; 2V_d t^{1/2} (\pi K_z)^{-1/2} \; - \; EPt \; (\Delta z)^{-1}\right]}{\pi \; \sigma_y \; (2 \; K_z t)^{1/2} \; \overline{u}} \; \exp -y^2/2(\sigma_y)^2 \; . \qquad (16)$$

Note that the value of χ_g used in Eqs. (6) and (11) is obtained from Eq. (16).

Typical deposition parameter values now being used in the model are:

$V_d = 3\times10^{-3}$ m/sec;

$E = 4.2\times10^{5}$ (by volume);

$P = 3.2\times10^{-8}$ m/sec; and

$\Delta z = 4000$ m.

Trajectories starting at a specified source point are printed on a gridded map, with grid spacing and area coverage selected by the user. Ground-level air concentration and deposition amounts are calculated for each grid box along and normal to each trajectory segment. The calculation normal to the trajectory is terminated at the 4 σ_y distance. Trajectories of duration up to 10 days may be started four times per day for a month, season, or year. Calculated concentrations from all trajectories are accumulated in each grid box and averaged over the chosen time period. A map is printed with coded mean air concentration values (for example, 2E = 2×10^{-21}) in each grid box, as illustrated in figure 1 for a hypothetical source in Illinois. The pattern of mean annual air concentrations is shown for a uniform emission rate totaling 1 mCi/year and assuming no deposition. When deposition parameter values are supplied as input, a second air concentration map is plotted which takes depletion by wet and dry deposition into account.

Figure 2 shows the air concentration map for the same source as for figure 1, but using the deposition parameter values listed above. A third map provides the calculated surface deposition pattern (wet and dry deposition combined) as shown in figure 3.

3. DIFFUSION MODEL FOR SHORT-TERM CONCENTRATIONS

The diffusion-deposition model described in section 2 was designed primarily for "climatological" applications where estimates of long-term average air concentrations and deposition patterns are required. For estimates of short-term (daily or twice daily) air concentrations at specific points of interest a more precise computational technique is desired. The diffusion model for short-term concentrations uses a series of instantaneous "puffs" to simulate a continuous emission. This model is better able to account for the distortion of a plume in a space-and-time varying wind field. When a trajectory loops or stagnates, for example, the puff model is superior to the continuous plume formulation which is strictly valid only for steady-state wind conditions.

The puff model is also more suitable for verification studies using an existing variable point source and where short-term air samples are taken at selected locations.

3.1 Puff Diffusion

Trajectories are started at 6-hour intervals and an instantaneous puff is transported along each trajectory and diffused according to the Gaussian

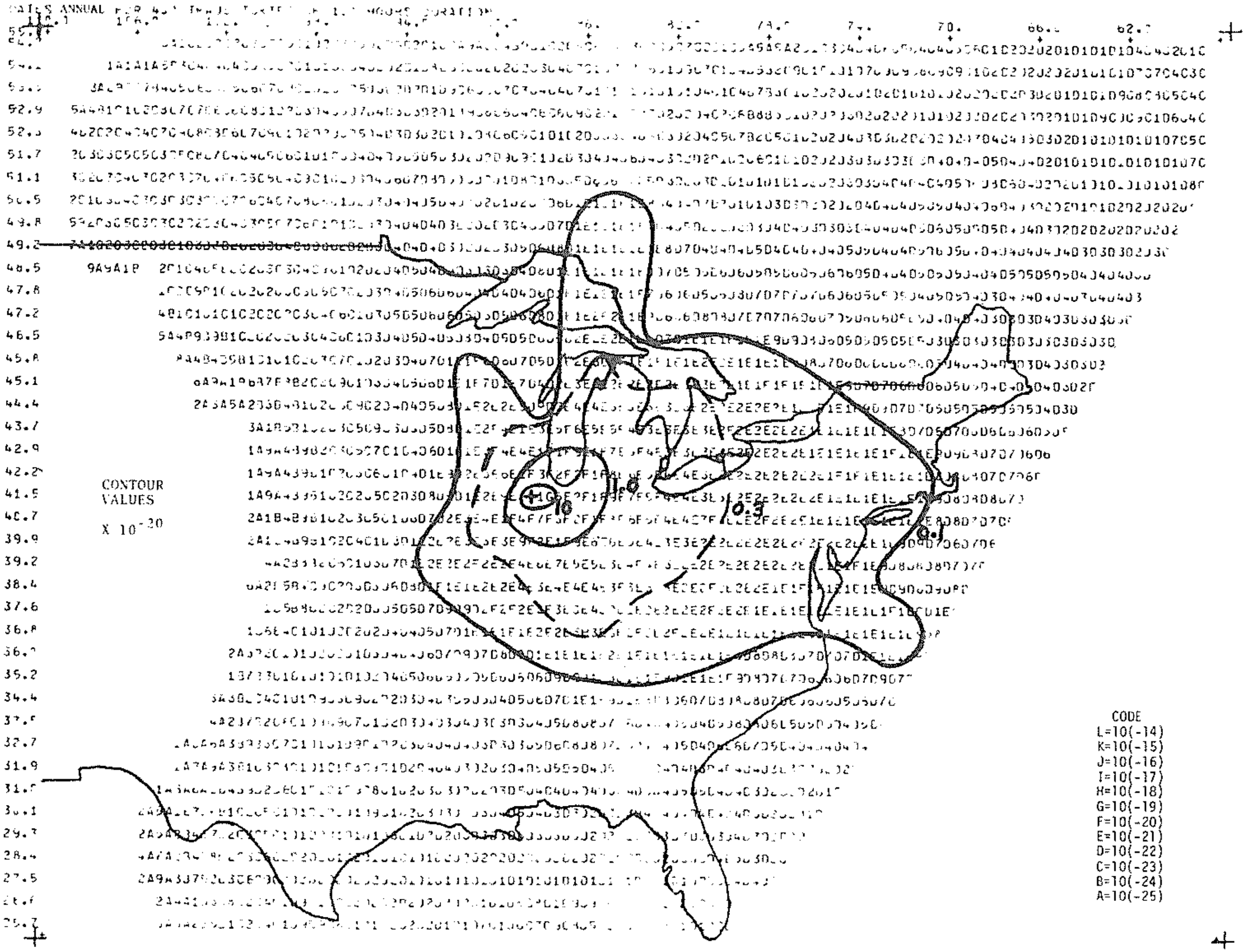

Figure 1. Map of coded mean annual ground-level air concentrations (Ci/m^3) based on trajectories for one month out of each season. Assumed emission rate is 1 m Ci/year.

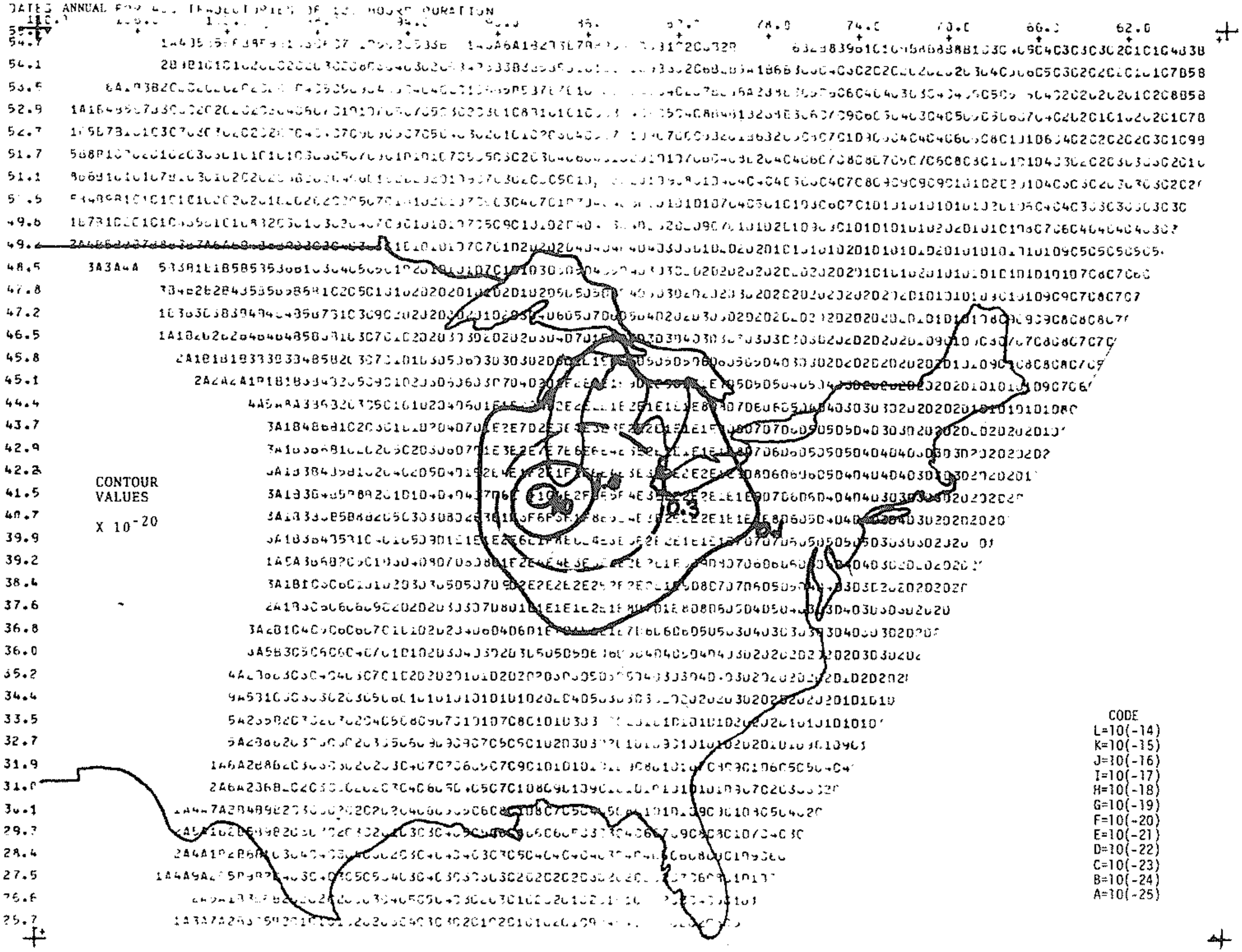

Figure 2. Mean annual air concentrations (Ci/m^3) with depletion by wet and dry deposition.

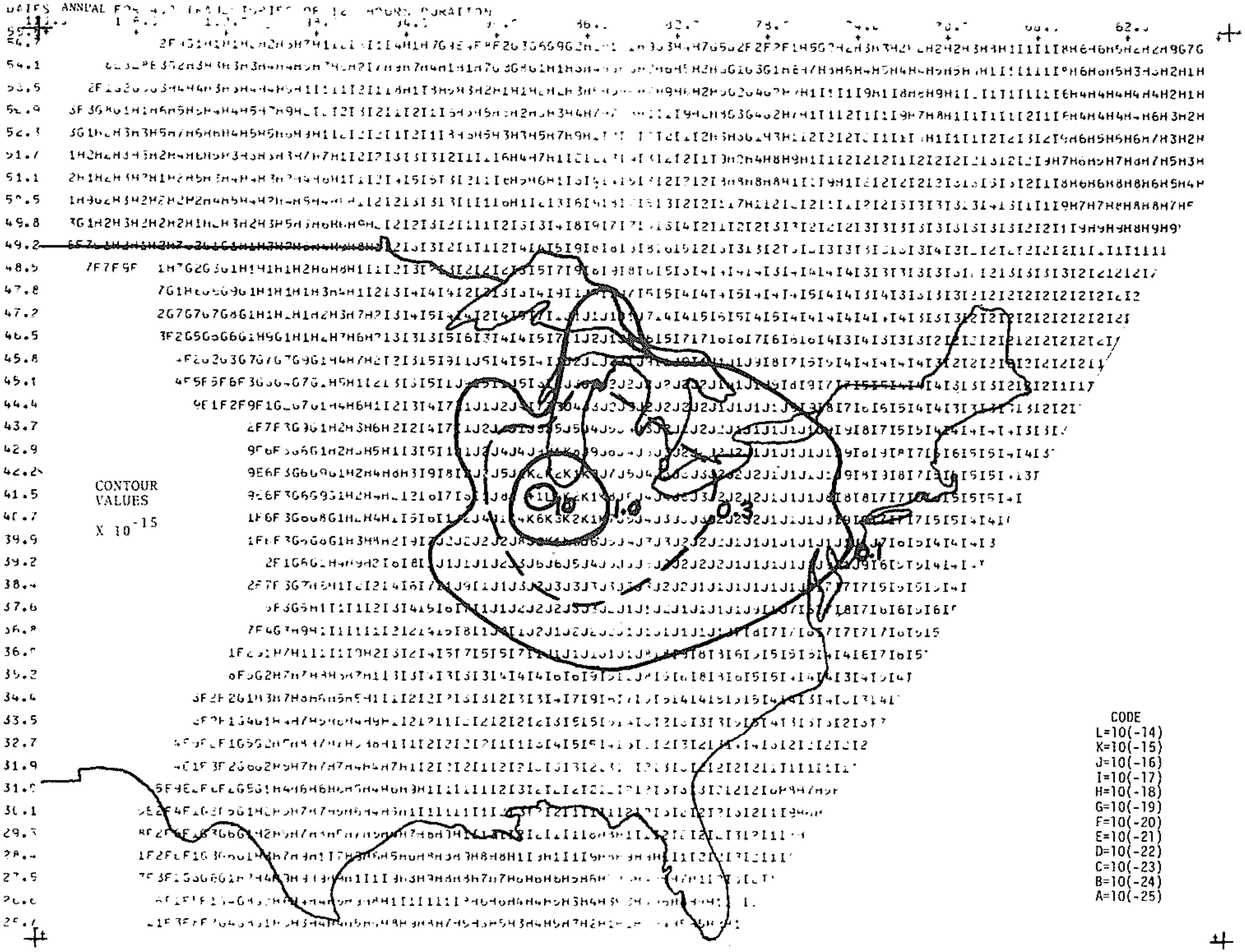

Figure 3. Total annual wet and dry deposition (Ci/m^2).

equation

$$X_g = \frac{2\,Q}{(2\pi)^{3/2}\,(\sigma_H)^2\sigma_z}\ \exp\,(-R^2/2\,\sigma_H{}^2) \qquad (17)$$

where X_g = ground-level air concentration, Q = total emission during the time interval represented by the trajectory (i.e., 6 hours for trajectories starting at 6-hour intervals), $\sigma_H = \sigma_x = \sigma_y$ = horizontal standard deviation of the puff, and R = distance (meters) from puff center to a sampling point.

It is assumed that σ_H, in meters, equals 0.5 times the travel times in seconds (see discussion of Eq. 5). The vertical standard deviation of the puff, σ_z, is obtained from Eq. (2).

An option provides for a uniform distribution through a specified mixing layer depth, L, instead of a Gaussian distribution in the vertical. With this option, the ground-level concentration is obtained from

$$X_g = \frac{Q}{2\pi(\sigma_H)^2\,L}\ \exp\,(-R^2/2\,\sigma_H{}^2). \qquad (18)$$

The distance, R, from the center of a puff to each sampling location is determined for the mid-point of each 3-hour trajectory segment and air concentrations at the sampling stations are calculated from Eq. (17) or (18). Concentrations are calculated only when $R \leq 4\sigma_H$. Concentrations from all trajectory segments within $4\sigma_H$ are stored in the proper sampling time period (one or two periods per day) at each sampling station. Figure 4 shows a one-day portion of a trajectory in relation to a sampling station. To

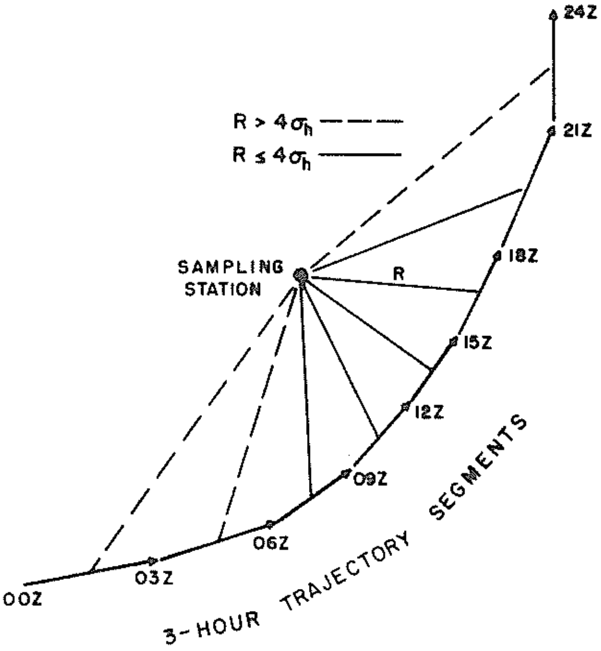

Figure 4. Trajectory segments in relation to a sampling station.

illustrate the procedure, we will assume two 12-hour sampling periods per day: 00Z to 12Z and 12Z to 24Z. The two 3-hour segments from 00Z to 06Z are assumed to lie beyond $4\sigma_H$, and these concentrations are not calculated. The segments from 06Z to 21Z do fall within the $4\sigma_H$ distance. Calculated concentrations for the 06 to 09Z and 09-12Z segments contribute to the 00Z to 12Z sampling period while the concentrations for the next 3 segments contribute to the 12Z to 24Z period. The last segment again lies beyond $4\sigma_H$ and no concentration is calculated. Contributions to each sampling period from all other trajectories would be similarly calculated and stored.

The model provides an option to determine R and calculate concentrations at more frequent intervals than 3 hours. A one-hour interval is recommended for sampling stations beyond about one-day's travel from the source. Stations closer to a source may require more frequent calculations to obtain a representative average concentration. The average concentration in a sampling period is obtained by summing all concentrations and dividing by the number of puff sampling intervals in a sampling period. For example, if the sampling period is 12 hours and puffs are sampled every hour, the calculated concentrations are divided by 12.

An option is also provided to linearly interpolate additional trajectories between those started at 6-hour intervals. The use of trajectories started at 3-hour intervals is recommended for calculating short-term concentrations beyond one day's travel.

3.2 Model Output

A listing for each sampling station gives the calculated mean air concentration for each sampling period and a break-down of the contributions from individual trajectories to each period. As shown in table 1, each sampling station is identified by call letters or numbers (e.g., DSM identifies Des Moines, Iowa). The sampling period is identified by date (and time interval,

```
STATION DSM
JAN75  MEAN  CONTRI- (DATE
DATE   CONC  BUTIONS  HOUR)
  21    112
             6.47E+00(1803)
             9.01E+00(1809)
             7.01E+00(1900)
             1.31E+01(1800)
             8.04E+00(1418)
             7.59E+00(1615)
             7.75E+00(1721)
             7.82E+00(1618)
             1.40E+01(1806)
             1.97E+01(1812)
```

Table 1. Mean air concentration and individual trajectory contributions for a one-day sampling period.

e.g., 00Z - 12Z, if less than 24 hours). Contributions from individual trajectories are identified by starting date and time (e.g., 1803 indicates the 03Z trajectory on the 18th day of the month). Space is provided to print the ten highest contributors. In the notation used here the number following the "E" indicates the power of ten, e.g., 1.97E + 01 indicates 19.7. Since the individual contributions have been divided by the time factor (number of puff sampling intervals per sampling period) the average concentration is simply the sum of all contributions. Note that the average concentration, 112 in this case, may be larger than the sum of the listed contributions if more than 10 trajectories contribute to a sampling period. Also note that puffs leaving a source on different days may contribute to the same period.

4. ACKNOWLEDGEMENT

This work was supported by the USAF Technical Applications Center and the Division of Biomedical and Environmental Research, Energy Research and Development Administration.

5. REFERENCES

Part II

Engelmann, R.J., 1970: "Scavenging Prediction Using Ratios of Concentrations in Air and Precipitation," Proc. Symposium on Precipitation Scavenging, AEC Symposium Series 22, pp. 475-485.

Heffter, J.L., 1965: "The Variation of Horizontal Diffusion Parameters with Time for Travel Periods of One Hour or Longer," J. Appl. Meteorol. 4 (1): 153-156.

Machta, L., G.J. Ferber, and J.L. Heffter, 1974: "Regional and Global Scale Dispersion of Krypton-85 for Population-Dose Calculations," Proc. Symposium on the Physical Behavior of Radioactive Contaminants in the Atmosphere, IAEA, Vienna, pp. 411-425.

Turner, D.B., 1970: Workbook of Atmospheric Dispersion Estimates," U.S. Environmental Protection Agency, Office of Air Programs Report No. AP-26, Research Triangle Park, North Carolina.