Tracer Verification of Trajectory Models

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ABSTRACT

Perfluorocarbon tracer data collected during the Cross Appalachian Tracer Experiment (CAPTEX '83) are used to determine the accuracy of three trajectory models: an isentropic, an isobaric, and a three-dimensional sigma model. The root-mean-square separation between model trajectories and trajectories derived from the surface tracer concentration is used to evaluate the models and assess the validity of isobaric, isentropic, isosigma, and mean transport vector assumptions. The root-mean-square data suggest that wind flow corresponding approximately to the low to middle boundary layer is the most appropriate for simulating the transport of boundary layer pollutants, and that the isentropic and isosigma transport assumptions are more realistic than the isobaric assumption. The results also indicate that synoptic type and the diurnal variation of mixing and wind shear within the boundary layer can affect the magnitude of root-mean-square separation between tracer trajectory and transport model trajectories. The uncertainty of the trajectory error suggested by the root-mean-square separation is approximately 50 km. Comparison of the tracer study with a theoretical study suggests that surface tracer data are useful for quantifying the magnitude of error in trajectory model calculations of boundary layer transport.

1. Introduction

Air parcel trajectories are necessary for revealing source–receptor relationships in atmospheric transport and deposition. Because spatial and temporal resolution of meteorological observations limit the accuracy of trajectory calculations, experimental verification of transport models is essential. Several techniques have been employed to provide verification of trajectory models. The most common technique is the use of tetraooons (Hoecker, 1977; Pack et al., 1977; Clarke et al., 1983). Tetraoos, however, although designed to move on a constant-density surface, are subject to the problem of large vertical oscillations caused by dew and solar radiation. Lamb (1981) has shown large differences between tetraooon trajectories and fluid particle (such as air pollutant) trajectories in situations where large vertical velocities exist.

Atmospheric tracer systems have provided important information about dispersion and transport of fluid particles but they have not been used extensively for verification of trajectory models. Lamb, Lorenzen, and Shair (1978) and Lamb, Shair, and Smith (1978) used sulfur hexafluoride tracer data to determine the reliability of air parcel trajectories constructed from meteorological data obtained in regions characterized by complex coastal meteorological conditions. Fowler and Barr (1983) released heavy methane tracers to test a simple diffusion model applied in conjunction with long-range trajectories produced by NOAA Air Resources Laboratory.

Walmsley and Mailhot (1982) used analytically specified nondivergent flow to evaluate the accuracy of long-range transport models. Their idealized flow patterns provide good qualitative information but do not allow for substantial trajectory model assessment. Recently, Kuo et al. (1985) employed a mesoscale predictive model to investigate the uncertainties of trajectory model computations. Assuming that the model simulation represented the “true” atmosphere, they generated a data base that allowed them to evaluate comprehensively the impact of spatial and temporal resolution, and of simplifying assumptions, on the accuracy of trajectory models.

In this study we use perfluorocarbon (perfluoromonomethyl-cyclohexane: C₃F₁₄) tracer data, available from the Cross Appalachian Tracer Experiment (CAPTEX '83), to evaluate three trajectory models designed for simulating long-range transport. They are the NCAR isentropic model, a more conventional isobaric model, and a three-dimensional sigma model developed jointly by the National Center for Atmospheric Research (NCAR) and Pennsylvania State University. More specifically, the tracer data are used to assess the

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accuracy of boundary layer trajectories derived from the models.

During September and October 1983, there were five tracer releases from Dayton, Ohio, and two releases from Sudbury, Ontario (see Ferber et al., 1986). Both ground and aircraft samples were collected. The aircraft samples provide very useful information about the vertical and horizontal structure of the plume at selected times and locations, but they are not used in this study because the methodology employed here requires a data base that is somewhat homogeneous in space and time.

Automatic sequential air samplers were operated at over 80 sites in the northeastern United States and southeastern Canada. Most samplers were programmed to take six consecutive 6-h samples (total duration of 36 h); however, sites closest to the release point generally took 3-h samples (18 h duration) for better definition of the plume. The surfac sampling distribution is shown in Fig. 1. Release sites are designated with an “R”. The sampling locations are arrayed in arcs (with respect to the Dayton release point) at approximately 100 km intervals at distances between 300 and 1100 km. The spacing of sample sites along each arc increases linearly with distance from Dayton because the intent was to resolve (from Gaussian theory) two-plume standard deviations. The density of sites on the 800-km arc is doubled to provide greater detail in that region. Several additional sites are placed just north of Lake Ontario to provide better measurement of plumes originating from the Sudbury release point. The overall mean distance between site locations is ∼80–90 km.

The tracer was released at ground level over a 3-h period on days when the lower-atmospheric wind flow was forecast to carry it over the sampling network. The synoptic flow pattern for the Dayton releases was influenced by low-level anticyclonic circulation over the southeastern United States. The wind flow over the network was generally from the west-to-southwest direction and relatively little precipitation occurred. The Sudbury releases followed passage of cold fronts associated with upper-level troughs. The circulation to the rear of the fronts produced northwesterly wind flow over the network. Some precipitation occurred along the frontal zone, particularly for the first Sudbury release. The Dayton releases were during the early afternoon to allow good vertical mixing of the tracer. The Sudbury releases were at night, but the meteorological conditions probably provided good vertical mixing (see Ferber et al., 1986).

In all, 1490 surface tracer samples are objectively analyzed to a grid. Eighty-one percent are 6-h samples, the remaining are 3-h samples. Since most samples are of 6-h duration, we combined (in most instances) sequential 3-h samples in order to provide a data base of uniform sampling length for the analysis. Table 1 gives the location, date, and time for the releases and lists the sample times and number of samples that are objectively analyzed for each release. Sample data from five consecutive 6-h sampling periods are analyzed for releases 1 through 5, and three consecutive 6-h sampling periods are analyzed for release 7. Sample data from release 6 are not used because the amount of release was small and the total sampling time short in

Fig. 1. Approximate location of surface sampling sites for CAPTEX tracer measurements. Release locations are designated with an “R”.
duration. Approximately 70% of the samples show a zero concentration. They are included in the objective analysis because they help define the lateral boundary of the plume.

In section 2, we describe and evaluate objective analysis techniques for analysis of tracer data. In section 3, we present examples of the objectively analyzed plumes and tracer-derived trajectories and discuss the method used for deriving trajectories from the tracer concentration distribution. A description of the trajectory models is given in section 4. In section 5, we give examples of the model trajectories and assess their accuracy using the tracer derived trajectories. We also discuss how uncertainties in the tracer concentration analysis and tracer-derived trajectories impose a limitation on the use of tracer data for verification of trajectory models. Our conclusions are given in section 6.

2. Objective analysis techniques for tracer data

The purpose of objective analysis is to use numerical methods for transforming data from irregularly spaced observations into meaningful data at regularly spaced intervals. The most widely accepted methods are grid point techniques (Haagenson, 1982) which use the observed values to correct errors in a gridded first-guess field that is approximated from the observations or from another dataset. A standard procedure is to analyze the “difference” fields, i.e., the difference between the observed values and the interpolated first-guess values at the observation locations. The corrections necessary to produce the final analysis are obtained (for each grid point) by multiplying the differences by weighting coefficients that are dependent on the distance between the grid points and the surrounding observations.

Important considerations for objective analysis are determination of appropriate grid point spacing, influence range of observations (radius of influence), and the technique used to calculate the most appropriate (optimum) weighting coefficients.

Two of the most frequently used objective analysis methods are the Cressman (1959) technique and “optimum interpolation” (Gandin, 1963). In this section we briefly describe these methods and present results of sensitivity tests designed to determine the grid resolution, radius of influence, and weighting coefficients that provide the best analysis of the CAPTEX surface tracer data.

a. Cressman analysis method

We employ a Cressman analysis to conduct sensitivity tests for determining the most satisfactory grid point interval and radius of influence, RI. The Cressman technique uses a first-guess field and explicitly assigns weighting coefficients to the difference values (observed-minus-interpolated first-guess values) at the observation locations. The first-guess field is generated by assigning each sample-site measurement to the nearest grid point and then applying a heavy four-point smoother. The first-guess fields for tracer data are of lower quality than those for meteorological data because predictive model data are not available and physical relationships with other variables are not established. The required interpolation of grid point values to the sample site (observation) locations is performed using a 16-point overlapping parabolic fit (described by Koehler, 1977). The two-dimensional interpolation in the 4 × 4 grid-square surrounding each observation location involves a series of one-dimensional interpolations in the x and y directions. Instead of fitting a third-order polynomial to four successive data points a, b, c, d, two parabolas are fitted to the 3-point datasets a, b, c and b, c, d. They are then combined into one curve by taking a weighed average.

The basic Cressman procedure is as follows: Given n observations of the difference variable, D_k, at n observation locations (k = 1, n) within influence radius RI and distance d_i from grid point i, we can calculate the correction D_i to the value at grid location i from

\[ D_i = \frac{\sum_{k=1}^{n} W_k^2 D_k}{\sum_{k=1}^{n} W_k}, \quad (1) \]

where the weighting coefficients, W_k, are given by the distance-dependent weighting function

<table>
<thead>
<tr>
<th>Release</th>
<th>Site</th>
<th>Release date</th>
<th>Period (UTC)</th>
<th>Sample periods</th>
<th>Number of samples</th>
<th>Midtime first sample period</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Dayton</td>
<td>18 Sept</td>
<td>1700–2000</td>
<td>5</td>
<td>48</td>
<td>18/2200</td>
</tr>
<tr>
<td>2</td>
<td>Dayton</td>
<td>25 Sept</td>
<td>1700–2000</td>
<td>5</td>
<td>32</td>
<td>26/0600</td>
</tr>
<tr>
<td>3</td>
<td>Dayton</td>
<td>2 Oct</td>
<td>1900–2200</td>
<td>5</td>
<td>48</td>
<td>03/0300</td>
</tr>
<tr>
<td>4</td>
<td>Dayton</td>
<td>14 Oct</td>
<td>1600–1900</td>
<td>5</td>
<td>85</td>
<td>15/0000</td>
</tr>
<tr>
<td>5</td>
<td>Sudbury</td>
<td>26 Oct</td>
<td>0345–0645</td>
<td>5</td>
<td>0</td>
<td>26/1100</td>
</tr>
<tr>
<td>7</td>
<td>Sudbury</td>
<td>29 Oct</td>
<td>0600–0900</td>
<td>3</td>
<td>76</td>
<td>29/1600</td>
</tr>
</tbody>
</table>
\[ W_k = \frac{(Rl)^2 - d_k^2}{(Rl)^2 + d_k^2}. \] (2)

Successive scans using decreasing RI can be employed, with RI ranging from a maximum of \( \sim 4d \) to \( d \), where \( d \) is the mean distance between observation locations.

b. Sensitivity to grid point resolution and radius of influence

Two criteria are used to determine the grid point resolution required to extract the most information from the irregularly spaced tracer observations: 1) the grid point interval required to minimize the root-mean-square (rms) difference between the observed and analyzed tracer concentration at the observation locations; and 2) the interval required to minimize the rms difference between the area-averaged observed and analyzed values in the vicinity of (200 km radius) each location. The normalized rms difference curves for both criteria are shown in Fig. 2. The curves are derived from a “single-scan” (Cressman analysis (RI = 200 km) using data from ten CAPTEX sampling periods (tracer releases 1 and 2). Since minimizing the rms difference at the observation location maximizes the area-averaged rms difference, and vice versa, we suggest that the optimum grid interval for simultaneously satisfying both criteria is the intersection of the curves (\( \sim 65-70 \) km).

The same criterion is employed to determine the most appropriate influence radius, RI. The normalized rms curves shown in Fig. 3 are again derived from a single scan Cressman analysis using the optimum grid point resolution determined from the previous sensitivity study. The rapid increase in rms difference at the observation location when RI is <80 km is because \( d \) (the mean distance between observation locations) is \( \sim 80-90 \) km. The intersection of the curves suggests an optimum value for RI of \( \sim 150 \) km which is about 1.7 times \( d \). This value is in good agreement with the ratio of 1.6 determined by Stephens and Stitt (1970).

c. Sensitivity to variations in the Cressman technique

The application of the weighting function in (1) differs from the two more commonly reported Cressman methods, given by Cressman (1959) in the form

\[ D_l = \frac{\sum_{k=1}^{n} W_k D_k}{n}, \] (3)

and by Haltiner and Williams (1980) in the form

\[ D_l = \frac{\sum_{k=1}^{n} W_k D_k}{\sum_{k=1}^{n} W_k}. \] (4)

The form given in (1) is discussed by Benjamin and Seaman (1985).

We use data from 28 CAPTEX sampling periods (all releases and time periods) and apply the sensitivity criteria discussed in section 2b to determine the most effective Cressman technique for the tracer data analysis. The results of nine experiments are given in Table 2a. Experiment 1, designed to represent the simplest form of objective analysis, is a “nearest-neighbor” first-guess-only analysis. A light smoother is used for experiment 1, while a heavy smoother is applied to the first-guess fields in the other experiments. (A heavy smoother was used in order to maximize the sensitivity.) Experiments 2, 3, and 4 pertain to the Cressman method variations shown in Eqs. (1), (3), and (4), respectively. The grid resolution is 70 km (all subsequent experiments use 70-km grid resolution) and RI is 150 km. Cressman method [Eq. (1)] with a variable RI is used for experiments 5 and 6. In experiment 5, RI is a function of distance from the release point. It in-

![Fig. 2. Normalized rms difference (ten sampling periods) between observed and analyzed tracer concentration as a function of grid point interval.](image-url)

![Fig. 3. Normalized rms difference (ten sampling periods) between observed and analyzed tracer concentration as a function of the radius of influence, RI.](image-url)

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creases linearly from a minimum value of 100 km (at a distance of 400 km from the release point) to a value of 300 km at a distance of 1200 km from the release point. In experiment 6, RI is increased linearly from a minimum value of 100 km, at a distance of 300 km from the release point to a value of 400 km at a distance of 1200 km from the release point. The successive-scan (two scans) application of Cressman method [Eq. (1)] is used for experiments 7 and 8. In experiment 7, RI is set to 300 and 150 km, respectively. In experiment 8, RI is set to 200 and 100 km, respectively. In experiment 9, Cressman method [Eq. (4)] is used; otherwise it is identical to experiment 8. Three scans using Cressman method [Eq. (1)] (not shown) do not significantly improve the analysis.

The results shown in Table 2a suggest that, for surface tracer analysis, Cressman methods [Eq. (1)] and [Eq. (4)] are better than method [Eq. (3)] and successive scans improve the analysis. The results of experiments 5 and 6 indicate that increasing RI with respect to distance from the release point does not significantly improve the analysis.

d. Optimum interpolation method

Gandin (1963) proposed a statistical regression procedure to select the optimum interpolation (OI). The regression coefficients are determined from the condition that the rms error of the analyzed difference values at the grid points is minimized over a large number of datasets. A large amount of historical data is required to calculate properly the statistical parameters for all types of variables and geographical locations. The required correlation functions are usually modeled mathematically as a function of distance, $d$, between observations and grid points.

We can write (4) in different form as

$$D_i = \sum_{k=1}^{n} \tilde{W}_{k} D_k.$$  

(5)

The optimum weighting coefficients, $\tilde{W}_{k}$, are derived by minimizing the rms error of $(\overline{D_i - D_j})^2$, where $D_i$ is the true correction value at grid point $i$, and the overbar denotes an average. The minimum rms error condition generates a system of $n$ linear equations.

$$\sum_{k=1}^{n} \tilde{W}_{k} \overline{D_k D_j} = \overline{D_i D_j} \quad (j = 1, n),$$  

(6)

where $j$ and $k$ are observation locations, $n$ is the number of observations within influence range RI, and $\overline{D_k D_j}$ and $\overline{D_i D_j}$ are the covariances. If we assume that $\overline{D_i^2} = \overline{D_j^2} = \overline{D_k^2}$, we can write (6) in terms of a distance-dependent correlation function $\mu(d)$ as

$$\sum_{k=1}^{n} \tilde{W}_{k} \mu(d)_{kj} = \mu(d)_{ij} \quad (j = 1, n).$$  

(7)

The weights $\tilde{W}_{k}$ needed to solve (5) are obtained from the solution of (7) if an appropriate correlation function $\mu(d)$ is available. The correlation coefficients are determined from distance between observations and between grid point and observation.

An advantage of OI is that positioning of data points with respect to each other is considered. If two observations are located near the same line through the grid point, the more distant observation might be assigned a negative weight which can then allow the analyzed value to be greater than the maximum or less than the minimum observed values in its vicinity. A disadvantage of OI is the lack of historical data, particularly for tracer data, and computational expense. Also, even if historical tracer data are available, an appropriate correlation function might be difficult to derive.

e. Sensitivity to variations in OI technique and correlation function

Since we did not have historical tracer data to derive a correlation function, a Gaussian distribution correlation function and a damped cosine correlation function were selected to conduct sensitivity tests. The Gaussian function has the form

$$\mu(d) = C_1 \exp(-C_2 d^2),$$  

(8)

where $C_1 = 1.0$, $C_2 = 2.3/(RI)^2$, and $d$ is the distance. The value of $C_2$ specifies that the correlation $\mu(d)$ is 0.1 when the influence radius RI is equal to $d$. The damped cosine correlation function [used by Haengenson and Shapiro (1979) for objective analysis of meteorological parameters in a transport model] has the form

$$\mu(d) = C_3 \cos\left(\frac{\pi}{2} \frac{d}{RI}\right) \exp(C_3 d),$$  

(9)

where $C_3 = -1.5 \times 10^{-3}$.

The results of the sensitivity tests are given in Table 2b. A damped cosine correlation function is used for experiment 10 and a Gaussian correlation function for experiment 11. Comparison of the rms differences for experiments 10 and 11 with the rms differences for experiments 8 and 9 (Table 2a) indicates that the successive-scan Cressman method minimizes the analysis errors as effectively as the OI method. Perhaps the OI method would have worked better if a correlation function could have been derived from historical tracer data. Experiment 12 (identical to experiment 11 except for the second scan) suggests that successive scans are not appropriate for the OI method.

3. Tracer plume analysis and tracer-derived trajectories

A successive scan Cressman method (experiment 8, Table 2a) is employed to derive the tracer plume analyses needed for construction of the tracer trajectories.
TABLE 2. Summary of sensitivity experiments for the objective analysis of tracer data.*

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Analysis technique</th>
<th>Influence radius (km)</th>
<th>Rms difference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Observation location</td>
</tr>
<tr>
<td>a. Cressman Method</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>First guess only</td>
<td>150</td>
<td>32.2</td>
</tr>
<tr>
<td>2</td>
<td>Eq. (1) single scan</td>
<td>150</td>
<td>32.5</td>
</tr>
<tr>
<td>3</td>
<td>Eq. (3) single scan</td>
<td>150</td>
<td>37.2</td>
</tr>
<tr>
<td>4</td>
<td>Eq. (4) single scan</td>
<td>150</td>
<td>33.2</td>
</tr>
<tr>
<td>5</td>
<td>Eq. (1) single scan</td>
<td>100 → 300</td>
<td>29.7</td>
</tr>
<tr>
<td>6</td>
<td>Eq. (1) single scan</td>
<td>100 → 400</td>
<td>31.0</td>
</tr>
<tr>
<td>7</td>
<td>Eq. (1) two scans</td>
<td>300, 150</td>
<td>31.0</td>
</tr>
<tr>
<td>8</td>
<td>Eq. (1) two scans</td>
<td>200, 100</td>
<td>25.6</td>
</tr>
<tr>
<td>9</td>
<td>Eq. (4) two scans</td>
<td>200, 100</td>
<td>25.9</td>
</tr>
<tr>
<td>b. Ol Method</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Damped cosine-single scan</td>
<td>150</td>
<td>28.6</td>
</tr>
<tr>
<td>11</td>
<td>Gaussian-single scan</td>
<td>150</td>
<td>25.6</td>
</tr>
<tr>
<td>12</td>
<td>Gaussian-two scans</td>
<td>200, 100</td>
<td>22.4</td>
</tr>
</tbody>
</table>

* The rms differences (all releases and time periods) between observed and analyzed tracer concentration are given in parts of perfluorocarbon per 10^{15} parts of air by volume (femtoliters/liter).

Although the method used in experiment 9 is as effective for minimizing the rms differences as the method used in experiment 8, we selected that of experiment 8 because Benjamin and Seaman (1985) show it to be the best for analyzing the gradients of meteorological variables. The Cressman method is selected instead of the Ol method because, computationally, it is much less expensive. For the final analysis, the nearest-neighbor first-guess fields are refined before beginning the Cressman scans by using the observed-minus-interpolated first-guess concentration value at the observation location and a simple weighting function to improve the surrounding first-guess grid point values. The weights ranged from 1.0 at the observation location to zero at a distance of two grid point intervals.

a. Tracer plume analysis

The analysis of the tracer data is based on the assumption that each sample is a 6-h sample (only 23 of the 3-h samples cannot be combined to simulate 6-h samples), and the sample is the observed concentration at midtime of the 6-h sampling period (refer to Table 1). Eighty-one percent of the samples used conform to the beginning and ending of the designated (standard) sampling periods. Thirteen percent pertain to samples starting an hour or two prior to the beginning of a standard sampling period, and 6% start an hour or two after the beginning of a standard sampling period. Examples of objectively analyzed plumes for a Dayton release (release 1) and a Sudbury release (release 5) are shown in Figs. 4 and 5.

Since the samples are integrated over a 6-h period and do not all begin at the same time, the analyzed concentrations cannot be interpreted as the instantaneous distribution of the surface tracer concentrations.

If the mean wind speed is 7 m s^{-1}, the analyzed tracer plume could be elongated in excess of 150 km with respect to the true plume. In the next section, we will discuss how elongation of the tracer plume might also be related to vertical shear of wind speed in the boundary layer.

b. Derivation of tracer trajectories

The horizontal and temporal distribution of the analyzed concentrations for releases 1–5 and 7 are used to construct air parcel trajectories. The relationship between plume concentration at the surface and lower atmospheric transport has been investigated by Haagenson and Morris (1974). They used surface measurements on six different days in the St. Louis, Missouri pollutant plume (120 km downwind from the source) to show that the bearing of the surface plume, in a moderately mixed boundary layer, is often centered approximately halfway between the surface flow direction and a mean transport vector direction defined as

\[ \mathbf{V}_T = \frac{1}{H} \int_0^H \mathbf{V} \, dz, \]

where \( z \) is height, \( H \) the vertical thickness of the plume, and \( \mathbf{V} \) the horizontal wind velocity. The results of their limited study suggest that a trajectory representative of air parcel transport in the lower portion of the boundary layer (BL) can be inferred from the maximum concentration of surface tracer. In the same study, they also developed a horizontal advection model to illustrate how surface concentrations in a pollutant plume can be significantly elongated in the downwind direction due to increasing wind speed with height within the BL. In a later section, we use model-derived tra-
FIG. 4. Objectively analyzed plume concentration for the tracer release from Dayton, Ohio, 18 September 1983. Contour values are given in parts of perfluorocarbon per $10^{12}$ parts of air by volume (femtoliters/liter). Panels a, b, c, and d correspond to the mid-time of sampling time periods 1, 2, 3, and 4, respectively.

FIG. 5. As in Fig. 4, but for the tracer release from Sudbury, Ontario, 26 October 1983.
jectories to compare surface trajectories, upper BL trajectories, and $V_T$ trajectories during the CAPTEX plume transport periods. We also discuss some effects of the diurnal variation of mixing and wind shear within the BL.

Three tracer-derived trajectories are constructed (starting at midtime of the release period) for each CAPTEX release. Each trajectory is based on a different assumption. The assumptions are that the position of the trajectory parcel at the midpoint of each sampling period is 1) the location of the analyzed maximum concentration, 2) the location farthest from the release point where the analyzed value is at least 20% of the analyzed maximum concentration and 3) the density-weighted maximum concentration location ($I$, $J$) defined from the analysis as

$$
I = \frac{\sum_{i=1}^{m} \sum_{j=1}^{n} iC_{ij}}{\sum_{i=1}^{m} \sum_{j=1}^{n} jC_{ij}}, \quad J = \frac{\sum_{i=1}^{m} \sum_{j=1}^{n} jC_{ij}}{\sum_{i=1}^{m} \sum_{j=1}^{n} iC_{ij}}
$$

(11)

where $i$ and $j$ are the grid point indices, $C_{ij}$ is the analyzed concentration at location ($i$, $j$), $m$ the number of grid points in the $y$-direction, and $n$ the number of grid points in the $x$-direction. The $I$, $J$ locations are calculated to the nearest tenth of a grid point, whereas the positions corresponding to assumptions 1 and 2 are at the $i$, $j$ locations.

The density-weighted assumption is introduced as an alternative to the location of the analyzed maximum concentration because the 6-h integration sampling protocol often leads to multiple maximum concentration locations. Assumption 2 is employed to investigate the relationship between elongation of surface concentration in the downwind direction and increasing wind speed with height within the BL.

Variations among the tracer trajectories for release 5 are shown in Fig. 6. The use of assumption 2 (dashed line) moves the tracer trajectory parcel the fastest while use of assumption 3 (dotted line) leads to the slowest parcel transport.

The rms separation between tracer trajectories constructed using the density-weighted maximum-concentration location (assumption 3) and trajectories constructed using each of the other assumptions is shown in Fig. 7. The curves, derived from all releases, show the rms separation as a function of sampling time period (time since release). Time period 5 is not used because, for some releases, part of the tracer is outside the sampling network. It is somewhat surprising that trajectories constructed from the density-weighted position location (assumption 3) vary significantly from trajectories constructed using the analyzed maximum-concentration location (assumption 1). The rms separation is much greater than that which can be attributed to the calculation resolution differences. In section 5, we will show that assumption 3 is preferable to assumption 1 for derivation of tracer trajectories.

![Fig. 6. Tracer-derived trajectories (arrowheads are given in 6-h increments) for the release from Sudbury, Ontario, 26 October 1983. Trajectories are based on assumptions 1 through 3, section 3b. Solid line indicates construction based on assumption 1, dashed line on assumption 2, and dotted line on assumption 3.](image-url)
4. Trajectory models

Three trajectory models are used to simulate trajectories for comparison with the tracer trajectories. They are a two-dimensional isentropic model, a two-dimensional isobaric model, and a three-dimensional sigma model. The meteorological input for the models is provided by the National Meteorological Center (NMC). The data are the operational grid point analysis of height, temperature, wind, and humidity on ten standard pressure levels from 1000 to 100 mb, and the original rawinsonde observation (raob) data. The input grid is a latitude–longitude mesh with a resolution of 2.5°. The temporal resolution for the grid analysis and raob data is 12 h. Supplemental meteorological data that are available for the CAPTEX sampling periods are not used in this study.

a. Isentropic model

The isentropic model (described by Haagenson and Shapiro, 1979) assumes that air motions are dry adiabatic; i.e., they take place on surfaces of constant potential temperature (θ),

$$\theta = T(1000/P)^{3/2},$$

where T is temperature (Kelvin) and P is pressure (millibars).

The procedure to generate the analysis required for construction of isentropic trajectories consists of three steps:

1) The latitude–longitude grid data on P surfaces are horizontally interpolated (using the overlapping parabolic method referenced in section 2a) to the NMC polar stereographic grid. The NMC grid resolution of ~350 km is roughly equivalent to the station separation of raob locations in the United States.

2) Both the grid point and raob data are coordinate-transformed to an isentropic framework by a transformation procedure described by Duquet (1964). The vertical resolution for the θ levels is 1°.

3) The first-guess grid point fields (on θ surfaces) are enhanced with the raob data using the OI method discussed in section 2d and the statistically derived correlation function defined by Eq. (9). Historically, the NCAR isentropic model has always employed the OI method. In this study, isentropic trajectories are also constructed using the Cressman method to determine if replacement of the OI method with the less expensive Cressman method significantly affects the model trajectories.

Special consideration is given to the zone where a θ surface intersects the ground. In this case an underground continuation of the θ surface is defined and the parcel is transported using the surface winds.

A trajectory path r(t) is related to the wind velocity field V(r, t) through the differential identity

$$\frac{dr(t)}{dt} = V(r, t).$$

(13)

After a time interval $\Delta t = (t_i - t_0)$, the position vector r(t) of a parcel is defined by

$$r(t_i) = r(t_0) + \int_{t_0}^{t_i} V[r(t), t] dt.$$  

(14)

However, if $\Delta t$ is equal to 12 h (normally the temporal resolution of the input data), the numerical evaluation of (14) is subject to error. The numerical method most frequently used is to divide $\Delta t$ by n subintervals. A 12-h trajectory is then computed from

$$r(t_i) = r(t_0) + \frac{1}{n} \Delta t \sum_{k=0}^{n-1} V(r_k),$$

(15)

where V(r_k) are the linearly interpolated u and v wind components at r_k. The trajectory path is constructed from n straight line segments joining the (n + 1) position vector locations.

The NCAR isentropic model employs a different technique. First, an iterative scheme is used that converges toward a point r_i by satisfying the equation

$$[r_0 + V(r_0, t_0) \Delta t] - r_i = [r_i - V(r_i, t_i) \Delta t] - r_0.$$  

(16)

Equation (16), which can be considered as the vectorial equivalent of the trapezoidal approximation of an integral, is obtained by equating, in magnitude and direction, the deviation between the point r_i and the straight-line forward displacement $r_0 + V(r_0, t_0) \Delta t$ to the deviation between the point r_0 and the backward displacement $r_1 - V(r_1, t_1) \Delta t$. For the first iteration, $r_1$
is the straight-line forward displacement from \( r_0 \). For each subsequent iteration, only \( r_1 \) is changed. The trajectory path connecting points \( r_0 \) and the final location of \( r_t \) is constructed objectively (described by Merrill et al., 1986) by combining the arcs of two circles that are tangent, respectively, to the velocity vectors at \( r_0 \) and \( r_1 \). The length and the temporal midpoint of the combined arcs are determined from the wind speeds at \( r_0 \) and \( r_1 \). The trajectory construction for the first time period is modified if the trajectory start time is not a standard data-input time, or if a frontal passage occurs at the start location.

b. Isobaric model

The isobaric model assumes that air motions take place on surfaces of constant pressure. The procedure to generate the analysis required for construction of isobaric trajectories is as follows:

1) The NMC latitude-longitude grid data on \( P \) surfaces at mandatory levels are horizontally interpolated (using the overlapping parabolic method referenced in section 2a) to a high-resolution grid (70 km for this study) on a Lambert-conformal projection.

2) The horizontally interpolated (first-guess) data are then vertically interpolated to four additional, nonstandard pressure levels (950, 900, 800, and 600 mb) to provide higher vertical resolution.

3) The first-guess grid point fields (on \( P \) surfaces) are enhanced with the raob data using the successive-scan Cressman method discussed in section 2a.

The isobaric trajectory path is derived from the numerical evaluation of Eq. (15) with the time step \( \Delta t \) equal to 1 h.

c. Sigma model

In the \( \sigma \)-coordinate model, \( \sigma \) is defined as

\[
\sigma = \frac{P - P_t}{P_s - P_t},
\]

where \( P_t \) is the pressure at the ground and \( P_t \) is 100 mb. In this coordinate system, \( \sigma \) surfaces near the ground closely follow the terrain profile, and \( \sigma \) surfaces in the middle and upper troposphere tend to approximate isobaric surfaces. The vertical motion (\( \dot{\sigma} \)) is calculated using the continuity equation (Anthes and Warner, 1978). We note that since the raob location density is low, the calculation of \( \dot{\sigma} \) is at best an approximation. If \( \dot{\sigma} = 0 \), the model assumes that air motions follow the \( \sigma \) surfaces. The procedure to generate the analysis required for construction of \( \sigma \) coordinate trajectories is the same as that for the isobaric trajectories, except that the final isobaric analysis is vertically interpolated to 15 \( \sigma \) levels ranging from \( \sigma = 0.05 \) and \( \sigma = 0.995 \). Typically, the lowest five to seven \( \sigma \) levels provide the vertical resolution for the afternoon BL.

The trajectory is derived from the three-dimensional evaluation of Eq. (15), where \( V \) is the vector representation of \( u, v, \sigma \) and the time step is equal to 1 h. If \( \dot{\sigma} = 0 \), the trajectory is two-dimensional on isosigma surfaces.

Surface (near ground) trajectories will result when \( \dot{\sigma} = 0 \) and \( \sigma = 0.995 \). The surface wind analysis is derived from the raob observations since the model is not designed to use standard surface data. Mean transport vector \( [V_T, Eq. (10)] \) trajectories are also constructed with the \( \sigma \) model; \( V \) in Eq. (15) is then \( V_T \), a two-dimensional vector. In this study, the vertical thickness \( H \) relates only to the depth of the afternoon BL which is approximated from the vertical structure of \( \theta \) along the trajectory path. We are assuming that a significant amount of the tracer resides above any nocturnal inversion.

5. Comparison of model and tracer-derived trajectories

In this section, we present data showing the sensitivity of rms separation between tracer and model trajectories to variations in tracer trajectory construction technique, tracer analysis method, model level, model design, transport assumptions, and synoptic type.

The isentropic, isobaric, and \( \sigma \) models are used to derive trajectories for each release, except release 6, at four levels within the BL. Isobaric trajectories are constructed on pressure levels of 1,000, 950, 900, and 850 mb. Isentropic, isosigma, and three-dimensional (\( \sigma \) model) trajectories are constructed for parcels starting at levels corresponding roughly to near surface (\( \sigma = 0.995 \) for the \( \sigma \) model and ~ surface \( \theta \) level for the isentropic model), 950, 900, and 820 mb. The \( V_T \) trajectories are constructed by averaging six \( \sigma \) levels ranging from the surface to ~900 mb. The depth of the afternoon BL for the CAPTEX cases generally ranged between 825 and 900 mb. We simplified our \( V_T \) calculations by using 900 mb for all cases. Surface trajectories are constructed with the \( \sigma \) model using the analyzed surface winds.

a. Sensitivity to tracer trajectory construction technique

The rms separation between model trajectories and the tracer-derived trajectories discussed in section 3b was usually the smallest when using the density-weighted tracer trajectory technique (assumption 3, section 3b). Table 3 shows the rms separation (all releases, levels, and time periods) between model and tracer trajectories for each assumption for isentropic, three-dimensional, isosigma, and isobaric trajectories. We observe that the density-weighted tracer trajectories result in the smallest rms separation for all the models. Overall, the rms separation is ~11% greater for the maximum-concentration technique (assumption 1,
Table 3. The rms separation (km) between tracer and transport model trajectories for different tracer trajectory assumptions.*

<table>
<thead>
<tr>
<th>Model</th>
<th>Trajectory type</th>
<th>Assumption</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Isentropic</td>
<td>Isentropic</td>
<td>253</td>
</tr>
<tr>
<td>Isobaric</td>
<td>Isobaric</td>
<td>281</td>
</tr>
<tr>
<td>Sigma</td>
<td>Three-dimensional</td>
<td>270</td>
</tr>
<tr>
<td></td>
<td>Isosigma</td>
<td>277</td>
</tr>
</tbody>
</table>

* See text (section 3b) for definitions.

section 3b) than for the density-weighted technique, and ~20% greater for the leading-edge technique (assumption 2, section 3b) than for the density-weighted technique. If the data are limited to the lowest two model levels, the 11 and 20% values become 17 and 52% respectively.

The sensitivity study indicates that the highest-level model trajectories correlate more closely with the leading-edge tracer trajectories than with the density-weighted or maximum-concentration trajectories; thus we might assume elongation of the analyzed surface concentration due to increased wind speed with height. The smallest rms separation, however, is usually observed between the density-weighted tracer trajectories and low- to middle-level model trajectories.

b. Sensitivity to tracer plume analysis method

In this section the sensitivity of rms separation (between model trajectories and tracer derived trajectories) to three tracer analysis methods is investigated. The trajectory types selected are the three-dimensional and isentropic, at levels corresponding to a starting pressure of ~950 mb and near-surface, respectively. Data show that the rms separation is the smallest for those levels (see section 5c). The methods tested are 1) the first-guess analysis used for experiment 1 in Table 2a, 2) the single-scan Cressman analysis used for experiment 3 in Table 2a and 3) the multiscan Cressman analysis used for experiment 8 in Table 2a. Method 3 is the tracer analysis used for all other results presented in sections 3, 4, and 5.

The rms separation for the three-dimensional trajectories (all releases and time periods) is about the same for analysis methods 2 and 3. The rms separation difference (between analysis methods 2 and 3) is only 1 km with the density-weighted tracer trajectory technique and also 1 km with the maximum-location technique. The leading-edge technique is not used here. When analysis method 1 (first guess only) is used, the rms separation is increased 27 km (14%) with the maximum-location construction but is only increased 6 km (4%) with the density-weighted trajectory construction. When the isentropic model is used, the overall rms separation between the density-weighted tracer isentropic trajectories is no larger for the first guess analysis than for analysis methods 2 or 3. The results suggest that if density-weighted tracer trajectories are used for verification of trajectory models, a "high-quality" objective analysis of the surface tracer data might not be necessary. However, if maximum-concentration location trajectories are used, a good-quality tracer analysis seems desirable.

c. Sensitivity to trajectory model level

Table 4 gives the rms separation (all releases and time periods) between model and tracer trajectories at four different model levels for isentropic, three-dimensional, isosigma, and isobaric trajectories. The tracer trajectories are derived using the Cressman tracer analysis discussed in section 3 and the density-weighted construction technique (all subsequent sensitivity tests use the above tracer analysis method and pertain to density-weighted trajectories).

The data show that the rms separation is minimized at the lowest level (starting near the surface) for isentropic trajectories, at level two (950 mb) for isobaric trajectories, and also at level two (starting at ~950 mb) for the isosigma and three-dimensional trajectories. Since the values are an average over all releases, the level of minimum rms separation for any given release is not necessarily the level indicated in the table. The height coordinates for the isentropic trajectories constructed for releases 1, 2, and 3 reveal that the isentropic parcels ascended following release. Therefore, at least in these cases, most of the isentropic transport occurred at heights well above the surface. The three-dimensional (σ model) trajectories show less ascending motion for releases 1, 2, and 3 than that suggested by the isentropic model. Perhaps that is why level 2 (instead of level 1) is the level of minimum rms separation for the three-dimensional trajectories.

d. Trajectory model intercomparison

Figure 8 shows the rms separation (all releases) as a function of elapsed time since release for isentropic, three-dimensional, isosigma, isobaric, and surface trajectories. The level used for each trajectory type,

<table>
<thead>
<tr>
<th>Model</th>
<th>Trajectory type</th>
<th>Level</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Isentropic</td>
<td>Isentropic</td>
<td>148</td>
</tr>
<tr>
<td>Isobaric</td>
<td>Isobaric</td>
<td>246</td>
</tr>
<tr>
<td>Sigma</td>
<td>Three-dimensional</td>
<td>240</td>
</tr>
<tr>
<td></td>
<td>Isosigma</td>
<td>243</td>
</tr>
</tbody>
</table>

* Level 1 is the lowest level and level 4 the highest.
excluding $V_T$ and surface trajectories, corresponds to the level of smallest rms value, for each type, in Table 4. The isentropic trajectories exhibit the smallest rms separation while the surface trajectories show a very large rms separation. The large rms separation for surface trajectories suggests that surface winds should not be used to simulate pollutant transport (at least not surface wind data having the resolution of raob observation data). We also note little difference between the isosigma and three-dimensional rms curves. Reasons for rms separation reduction after 19 h (some curves) are discussed in subsection 5e.

Table 5 gives the rms separation and mean standard deviation for the dataset used in Figure 8 (all releases and time periods), and for the same set with release 7 excluded. The mean standard deviation is the mean value of the standard deviation for all releases at each time period. In addition, rms values for a “modified” isentropic model are also shown. In the modified version of the NCAR isentropic model, the OI objective analysis method is replaced by a multiscan Cressman analysis.

Note that exclusion of release 7 results in a significant decrease in rms and standard deviation values for the isobaric, three-dimensional, isosigma, and $V_T$ trajectories, particularly the $V_T$ trajectories. Reasons for the decrease are discussed in the following section.

e. Sensitivity to synoptic type and diurnal effects

The tracer release periods represent a very limited ensemble of synoptic situations. Table 6 shows the rms separation (all time periods) for each release for the trajectory types and levels given in Table 5. The synoptic patterns for releases 1 through 4 are similar; the flow pattern was influenced by anticyclonic circulation over southeastern United States. Very little precipitation was observed over the sampling network. The synoptic patterns for releases 5 and 7 were characterized by the passage of cold fronts associated with upper-level troughs (both tracer releases began shortly after frontal passage). Some precipitation occurred along the frontal zones. The isentropic and three-dimensional analysis show that the upper-level trough associated with release 7 produced strong—large scale—sinking motion to the rear of the surface cold front.

The mean value of the rms separation (excluding surface) for releases 1, 2, 3, and 4, where no cold frontal passage occurred, is $\sim 35$ km less than the value for release 5 and $\sim 105$ km less than the value for release 7. One possible reason for the rms difference, other than frontal related, is that releases 1, 2, 3, and 4 were during the day whereas releases 5 and 7 were at night. However, Ferber et al. (1986) suggest similar vertical mixing at time of release for all releases.

For release 7, we observe very large rms separation for all trajectory types except isentropic and surface. The height coordinates of the isentropic trajectories also indicate surface transport for the isentropic parcels. Perhaps the observed sinking motion along the tracer trajectory path limited the vertical extent of the tracer, and thus surface trajectories provided the best representation of the tracer transport. (The raob data along the trajectory path, however, do not clearly suggest limited vertical extent of the tracer; the temperature profiles reveal a near-adiabatic lapse rate up to at least 900 mb.) Since the height coordinates of the three-dimensional trajectories indicate transport between the surface and 950 mb, the rms separation pertaining to the three-dimensional trajectories is larger, like the other higher level trajectories. Figure 9 shows the variation of model trajectories for release 7. The isentropic,

* Modified isentropic, OI analysis is replaced with the multiscan Cressman analysis.
** Numbers in parentheses are the standard deviation.

### Table 5. The rms separation (km) between tracer and transport model trajectories at levels showing lowest rms values.

<table>
<thead>
<tr>
<th>Model</th>
<th>Trajectory type</th>
<th>All releases</th>
<th>With release 7 excluded</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isentropic</td>
<td>Isentropic</td>
<td>148 (54)**</td>
<td>151 (57)</td>
</tr>
<tr>
<td>Isentropic*</td>
<td>Isentropic</td>
<td>138 (62)</td>
<td>136 (65)</td>
</tr>
<tr>
<td>Isobaric</td>
<td>Isobaric</td>
<td>193 (93)</td>
<td>160 (66)</td>
</tr>
<tr>
<td>Three-dimensional</td>
<td>Three-dimensional</td>
<td>158 (81)</td>
<td>133 (62)</td>
</tr>
<tr>
<td>Sigma</td>
<td>Isosigma</td>
<td>165 (77)</td>
<td>138 (56)</td>
</tr>
<tr>
<td>$V_T$</td>
<td>171 (95)</td>
<td></td>
<td>133 (66)</td>
</tr>
<tr>
<td>Surface</td>
<td>271 (68)</td>
<td></td>
<td>280 (60)</td>
</tr>
</tbody>
</table>

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isobaric, three-dimensional, and surface trajectories are shown along with the density-weighted tracer trajectory. The model trajectory levels correspond to the levels used in Table 6. The observed vertical shear of wind (revealed from raob data) is reflected in the trajectories—the isobaric trajectory (950 mb) is at the highest altitude.

The large rms separation for release 3, relative to releases 1 and 2, might be partly due to the magnitude of vertical shear of wind direction in the BL. The angular separation between the lowest- and highest-level trajectories is largest for release 3. Also, the tracer concentration analysis for release 3 shows the most diurnal variation. (The diurnal variation is discussed later.) The large rms separation for release 4, relative to releases 1 and 2, is probably because first-guess grid point fields, normally provided by NMC, are not available for most of the analysis time periods. Release 4 is the only release that did not have first-guess fields for all of the analysis time periods.

Figure 10 is similar to Fig. 8 except that release 7 is excluded from the dataset. The curves in Fig. 10 show the expected increase in rms separation with elapsed time. In Fig. 8 (release 7 included in the dataset) a decrease in rms separation is observed for some curves after 19 hours of elapsed time. The decrease occurs because tracer data are not available beyond 19 hours for release 7. Consequently, the large rms separation, characteristic of the three-dimensional, isobaric, iso-
sigma and V_T trajectories for release 7, elevate the overall rms values out to (but not beyond) 19 hours elapsed time. Release 7 is the only release where tracer data are not available for at least four of the 6-h time periods.

<table>
<thead>
<tr>
<th>Table 6. The rms separation (km) between tracer trajectories and transport model trajectories for each release.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>Isentropic</td>
</tr>
<tr>
<td>Isentropic*</td>
</tr>
<tr>
<td>Isobaric</td>
</tr>
<tr>
<td>Sigma</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Mean (excluding surface)</td>
</tr>
</tbody>
</table>

* Modified isentropic.
The influence of the diurnal variation of mixing and wind shear within the BL is the most noticeable for release 3 where a distinct increase in the spatial extent of the analyzed surface concentration is observed (Fig. 11) between time period 2 (a nighttime sampling period) and time period 3 (a daytime period). The orientation of the plume axis also changes significantly. The analysis suggests that part of the tracer was transported above the nocturnal inversion (where wind speeds are greater and wind direction different than that at the surface) during the second time period and then was mixed downward to the surface during the third time period. The accuracy of the analysis north of Lake Erie, however, is limited due to inadequate station resolution and missing data. The length of the tracer trajectory segments for release 3 are also much shorter at night than during the day. The diurnal influence for the other releases is not as discernible.

Diurnal effects are also suggested by the rms separation curves in Fig. 10. We note that the surface rms values are not significantly larger than the rms values for the other trajectory types until time period 3. Most of the tracer samples were daytime samples for time period 3 and nighttime samples for time period 2.

f. Limitations on the use of tracer data for trajectory model verification

Uncertainties in the tracer concentration analysis and tracer-derived trajectories impose a limitation on the use of tracer data for verification of trajectory models. Factors contributing to the uncertainty of the analysis are 1) the tracer samples are integrated over a 6-h period, 2) samples pertaining to the same time period do not all begin at the same time and 3) the first-guess analysis is of low quality because predictive model data are not available. Factors contributing to the uncertainty of the tracer-derived trajectories, in addition to the uncertainty of the analysis, are 1) the trajectories are constructed from a two-dimensional surface concentration distribution that is influenced by three-dimensional BL processes such as vertical mixing and wind shear, and 2) different assumptions regarding the position of the trajectory parcel with respect to the tracer concentration distribution lead to significantly different trajectories.

A rough approximation for the magnitude of difference (uncertainty) between the "actual" trajectory error and that suggested by the rms separation is $\sim 50$ km. This estimate is based on extrapolation, to zero hours elapsed time, of the rms separation curve shown in Fig. 12. The rms separation is the average of the rms separation values used in Fig. 10, excluding the surface trajectories. In view of the uncertainties in the tracer analysis and tracer trajectories, the differences in rms separation among model trajectory types shown in Table 5 (except for the surface and isobaric transport) are probably not significant. However, comparison of the isentropic and modified isentropic rms values suggests that the OI analysis method in the isentropic model can be replaced with the less expensive Cressman method.

g. Uncertainty in trajectory model calculations

The rms separation curve in Fig. 12 represents an estimate, in a Monte Carlo sense, of the error in long-range transport calculations (at least for the models used in this study). Since the mean total transport distance of the tracer trajectory parcel at 24 h after release is $\sim 800$ km, a mean trajectory error of $\sim 200$ km is suggested for 800 km transit distance.

Kuo et al. (1985) used the results from a mesoscale model simulation of a developing cyclonic storm to investigate the accuracy of trajectory models. They constructed three-dimensional trajectories from the model data and assumed that the predictive trajectories were the "true" atmospheric trajectories. The model data were then degraded to mimic the temporal and spatial resolution of the data routinely available as input to trajectory models. Trajectory computations were repeated and compared with the "true" trajectories to determine the magnitude of mean absolute trajectory errors expected for three-dimensional trajectory model computations. Using the degraded data, they also constructed trajectories on isentropic, isobaric, and isosigma surfaces in order to determine the effect of simplifying assumptions on the magnitude of the trajectory errors.

The difference in mean absolute trajectory error among trajectory types (isobaric, isentropic, isosigma, and three-dimensional) in the theoretical study is comparable to that shown for the difference in rms separation among trajectory types in the tracer study. The
solid curve in Fig. 13 shows the mean absolute trajectory error, in the low to middle BL, averaged for the theoretical calculations of isobaric, isentropic, isosigma, and three-dimensional trajectory errors. The tracer-derived rms separation curve from Fig. 12 is included (dashed curve) for comparison. The similarity of results obtained by using significantly different experimental design supports the usefulness of both studies for determination of the error in BL transport calculations.

6. Conclusions

Perfluorocarbon tracer data, available from the Cross Appalachian Tracer Experiment (CAPTEX '83), are used to evaluate three trajectory models designed for simulating long-range transport. They are an isentropic, an isobaric, and a three-dimensional \( \sigma \) model. During September and October 1983, there were five tracer releases from Dayton, Ohio, and two from Sudbury,
Ontario. Automatic air samplers were operated at over 80 sites in northeastern United States and southeastern Canada. The mean distance between sites is ~80–90 km.

Approximately 1500 surface tracer samples are objectively analyzed to a grid. Sensitivity studies indicate that the tracer analysis errors are minimized most effectively using a grid resolution of 70 km and influence range for the observations of 150 km. Sensitivity tests also show that a successive-scan Cressman analysis is preferable to the more costly optimum interpolation method.

Tracer trajectories are objectively constructed from the horizontal and temporal distribution of the surface tracer concentration, and rms separation between model trajectories and tracer derived trajectories is used to evaluate the models and assess the validity of isobaric, isentropic, isosigma, and $V_T$ (mean transport vector) assumptions. The smallest rms separation between model and tracer trajectories occurs when a density-weighted tracer trajectory technique is employed. Also, if the density-weighted technique is used, a high-quality tracer analysis might not be necessary for the model verification. The rms separation data suggest that surface wind trajectories should not be used to simulate the BL pollutant transport (at least not trajectories calculated from surface wind data having the resolution of raob observation data); wind flow corresponding to ~ low to middle BL is much more appropriate. In addition, the results suggest that the isentropic, $V_T$, and isosigma transport assumptions are more realistic than the isobaric assumption; results also indicate that synoptic type and the diurnal variation of mixing and wind shear within the BL can affect the magnitude of rms separation between tracer trajectory and transport model trajectories. However, since the tracer release periods represent a very limited ensemble of synoptic situations, we cannot demonstrate a significant relationship between synoptic type and rms separation.

Uncertainties in the tracer concentration analysis and tracer-derived trajectories impose a limitation on the use of rms separation between tracer and model trajectories to determine trajectory errors. In general, an approximation for the magnitude of difference (uncertainty) between the “actual” trajectory error and that suggested by the rms separation is ~50 km.

Comparison of the tracer study results with the results of a theoretical study suggests that surface tracer data are useful for quantifying the magnitude of error in trajectory model calculations of BL transport.

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Fig. 12. The average rms separation between tracer trajectories and transport model trajectories as a function of hours after tracer release. The average is computed from the data in Fig. 10 (surface values excluded). The dashed line extension of the curve is an extrapolation to the zero hours elapsed time.

Fig. 13. Mean absolute trajectory error (solid curve), as a function of time, averaged for the theoretical calculations of isobaric, isentropic, isosigma, and three-dimensional trajectory errors. The dashed curve is the rms separation curve from Fig. 12.

REFERENCES


