Statistical Interpretation of Pollution Data from Satellites

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The NIMBUS-G environmental monitoring satellite has an instrument (a gas correlation spectrometer) onboard for measuring the mass of a given pollutant within a gas volume. The present paper treats the problem: how can this type measurement be used to estimate the distribution of pollutant levels in a metropolitan area? Estimation methods are used to develop this distribution. The pollution concentration caused by a point source is modeled as a gaussian plume. The uncertainty in the measurements is used to determine the accuracy of estimating the source strength, the wind velocity, diffusion coefficients, and source location.

Nomenclature

c_y, c_z = horizontal and vertical dispersion parameters, respectively
H = height of source
K = instrument sensitivity
ℓ_y, ℓ_z = horizontal and vertical dispersion distances, respectively
M = information matrix
P = instrument output
Q = source strength
R = radius of view field
S = surface area of circular region
u = wind speed
V = volume viewed by sensor
W = weighting matrix
X, Y, Z = Earth-fixed reference system
x, y, z = reference system defined by source and wind
$\bar{x}$ = vector of parameters to be estimated
α, β = exponents in ℓ_y, ℓ_z equations, respectively
δ = residual
ϵ = measurement error
θ = wind direction angle
Λ = matrix of partial derivatives
$\sigma_{(\ )}$ = standard deviation of subscripted variable
Φ_i = i^{th} measurement
ψ = pollution concentration

Introduction

AN application of space technology to help improve the environment is the use of satellites to monitor air pollution. It is axiomatic that measurement is necessary for control of a process, and satellites offer the means of providing coverage over large areas to insure that environmental standards are met and maintained. NASA is presently developing a number of instruments which use gas spectroscopy to detect and measure pollutants within the Earth's atmosphere.[1] These instruments are suitable for use onboard satellites for remote sensing. One such satellite is the NIMBUS-G environmental monitoring satellite. Among the instruments to be carried by NIMBUS-G are spectrometers which will measure the total mass of a given gaseous species of pollutant, for example, methane (CH_4), sulfur dioxide (SO_2), nitrogen dioxide (NO_2), and carbon monoxide (CO), within a given volume of gas. Because "high" concentrations of these pollutants are small on an absolute basis (being measured in parts per million) to get an adequate signal from the instrument at orbital altitude it is necessary to give a rather large volume of gas. Thus, the signal from the instrument depends on the distribution of a pollutant species within a circular cone with its apex at the satellite and intersecting the ground with a circle of 20-50 km radius, depending on the final design of the instrument (see Fig. 1). As the satellite moves along its orbit, the instrument output varies according to the pollution within the volume viewed. One purpose of the NIMBUS-G is the determination of the large-scale (continental and global) distribution of atmospheric pollution. In addition, it will be necessary to obtain as much information as possible from the satellite concerning metropolitan scale distribution.

In the present paper, the problem is considered: How can satellite air pollution measurements of the type described above be used to help estimate the distribution of pollutant levels in a metropolitan area? In addition to the satellite measurements, one also has available information such as a pollutant concentration model, meteorological data, and source locations, all of which are imperfect. There may also be in situ point measurements within the area. The problem is formally similar to the orbit determination problem in that measurements are used in conjunction with a model of the process to estimate the state of the system and some of the important parameters. This paper presents a formulation for the statistical interpretation of air pollution measurements from satellites, for the inference of air pollution sources and levels within a metropolitan area.

Three regions of the problem of satellite pollution data interpretation are distinguished: the field of view of the instrument is large, same order of magnitude, or small com-

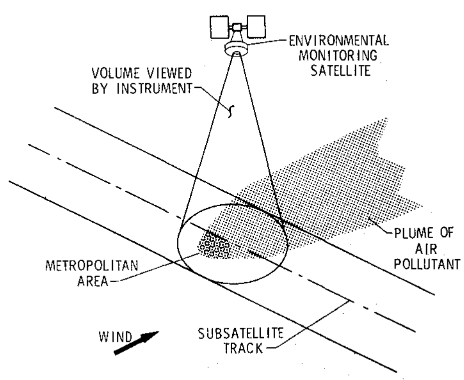

Fig. 1 Air pollution monitoring by satellite.

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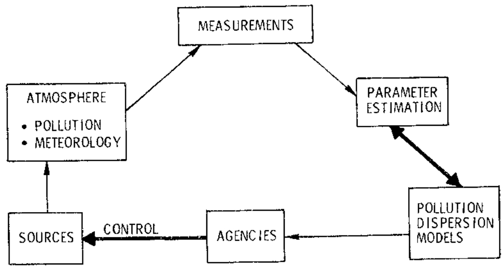

Fig. 2 Role of parameter estimation in environmental monitoring.

pared to the scale of pollutant distribution of interest. The present paper deals with the first regime. Here, the information from the instrument can only be interpreted with the aid of modeling; the desired level of detail is not present in the measurement alone.

The approach taken in this paper is to model the pollutant distribution such that it is expressed in terms of a small set of parameters: source strength and location, wind speed and direction, and dispersion coefficients. These parameters are then estimated by use of the satellite data and any other available data. The model parameters having been estimated, the pollution concentration field may be computed. In addition, parameter estimation techniques provide estimates of the accuracy with which the model parameters have been computed.

The role of parameter estimation in environmental monitoring is shown in Fig. 2. Measurements are made of atmospheric pollution and meteorological conditions. These measurements cannot be used directly in pollution dispersal models. Parameter estimation methods provide the vital link between the dispersal model and the monitoring which enable the measurements to be interpreted in terms of the pollution distribution. Once these hardware and software systems have been developed and demonstrated, they may then be turned over to the appropriate government agencies for providing information on the atmospheric pollution condition. These agencies at the local, state, and federal levels can then supply whatever control is desirable on the pollutant sources.

To demonstrate the application of parameter estimation techniques to interpretation of pollution data, only the simplest problem is considered. It is assumed that conditions are in steady state, thereby simplifying the problem conceptually. Also, as an arithmetic simplification a point source, uniform wind, and no sinks or scavenging processes are assumed. The simplicity of the treatment permits a number of important conclusions to be made which "physical reasoning" indicates are not invalidated by the simplicity of the model. Because of the scale of the problem, a city constitutes a point source.

Studies of this type should impact the design of pollution monitoring satellites, for example, in the tradeoff between instrument accuracy and field of view of the instrument. To get good accuracy from the instrument, it is necessary to have a large output, which requires a large field of view. With the large field of view, spatial resolution is lost. The study also aids in selection of data rate, by determining how many data are required and how many are adequate.

Analysis

A single gaseous species of atmospheric pollutant will be considered. The goal of the analysis is to estimate the concentration of the pollutant throughout the region of interest and the accuracy of this estimate, given measurements made by an instrument aboard a satellite. The problem will be analyzed in the following sequence. First, the nature of the satellite data will be considered, after which the model of the dynamics of pollution dispersal will be discussed. Next, the parameter estimation process is briefly reviewed and applied to the present problem.

The concentration of the pollutant at a point x,y,z will be denoted as $\psi(x,y,z)$, and will be assumed to be independent of time. The goal of the analysis is thus to estimate $\psi(x,y,z)$.

Satellite Data

In the present paper, it will be assumed that the output of the instrument is proportional to the total mass of pollutant within the viewing cone as shown in Fig. 1. Thus, the observation is modeled as

$$\Phi = K \int\int\int_V \Psi \, \mathrm{d}V + \epsilon \tag{1}$$

where Φ = instrument output, K = instrument sensitivity, ϵ = random error in measurement with zero mean and variance σ^2_{obs}, and the integral is taken over the cone. For an instrument using gas correlation spectroscopy, and depending on thermal absorption and emission by the pollutant species, there would be a weighting function in the integrand which would be approximately proportional to the difference in temperature between the gas at a point and the background. Also, if the pollutant were optically thick, the relation of instrument output to pollutant distribution would be more complicated. These refinements may be incorporated for a particular instrument when it becomes available. To present the application of statistical estimation to the satellite data, it will be assumed that the instrument signal is proportional to the total mass of pollutant viewed, as expressed by Eq. (1).

As the satellite moves along its orbit, the volume of gas which is viewed constantly changes. At regular intervals, data are recorded. Thus, the data consist of a set of numbers, Φ_i. It is obvious that this finite set of numbers alone does not uniquely determine the pollutant distribution ψ. The resolution of the ψ field which is possible from the data in the horizontal plane is well suited for continental and global scales. However, for metropolitan scale, the ψ field cannot be inferred from the satellite data alone, and metropolitan air pollution is of such concern that a method must be developed for using the data to estimate it.

The problem is approached by noting that the ψ field is not an arbitrary distribution, but is governed by the dynamics of pollutant dispersal. This is a considerable constraint on the ψ field. Thus, the satellite data are used in conjunction with a pollutant dispersal model to infer the pollutant distribution.

Pollution Dispersal Model

The dynamics of air pollution dispersal can be modeled in any of several ways. It has been observed that point sources have gaussian plumes whose lateral dispersions vary almost linearly with downstream distances from the sources, as discussed by Pasquill in Ref. 2. In the present paper, the pollutant concentration will be modeled following Refs. 2 and 3 as

$$\psi(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\tfrac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]$$
$$\times\left\{\exp\left[-\tfrac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\tfrac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \tag{2}$$

where Q = source strength, σ_y, σ_z = horizontal and vertical dispersion distances, respectively, u = wind velocity, and H = height of source. This equation is suitable for a steady-state source release at a height H into the atmosphere with uniform mean conditions. It is also assumed that there are no scavenging effects such as gas phase chemical reactions or absorption at the ground, and diffusion in the along wind direction is neglected. The ground is assumed to reflect the pollutant. The variations of σ_y and σ_z with downwind distance x from the source and with atmospheric stability are shown in Fig. 3-2 of Ref. 3. It is noted from that figure that very nearly

$$\sigma_y = c_y x^\alpha \tag{3a}$$

$$\sigma_z = c_z x^\beta \tag{3b}$$

where α is very near 1 and c_y and c_z are horizontal and vertical dispersion parameters, respectively. These parameters are a function of atmospheric stability.

To use this plume model, coordinate systems are defined as shown in Fig. 3. The $X-Y$ system is a basic earth-fixed reference system. The wind direction measured in this system is θ. The source location within the X-Y system is X_s, Y_s. The x-y system is defined with its origin at the source and the x axis parallel to the wind vector.

The parameters of this plume model are: source strength Q, horizontal and vertical dispersion parameters c_y and c_z, wind speed u and direction θ, and location X_s, Y_s. Given these parameters, the pollutant concentration ψ can be computed throughout the region by Eq. (2).

An alternative approach to dispersion modeling is to treat the atmospheric mixing as analogous to molecular diffusion, which results in the classical diffusion equation with advection. The solution to this equation for a point source in a uniform unbounded flow is a gaussian distribution, with the characteristic lateral dimension varying as $x^{1/2}$, where x is the distance downwind of the source. As is shown by Taylor[4] and Sutton[5] this dispersal rate is valid only if the characteristic scale of the turbulence is small compared to the lateral dispersion of the plume. Because of the spectrum of atmospheric turbulence at long wavelengths, the growth of the plume is more nearly linear, as discussed by Pasquill.[2]

The instrument output can now be computed in terms of the model and its parameters, by using Eq. (2) to express ψ in the integrand of Eq. (1). Thus, the computed output P is given by

$$P=K\int\int\int_V \psi \mathrm{d}V=\frac{KQ}{2\pi u}\int\int_S \frac{1}{\sigma_y\sigma_z}\exp[-1/2(\frac{y}{\sigma_y})^2]$$
$$\times\,(\int_{z=0}^{z=z_c}\{\exp[-1/2(\frac{z-H}{\sigma_z})^2]+$$
$$\exp[-1/2(\frac{z+H}{\sigma_z})^2]\mathrm{d}z)\,\mathrm{d}S \tag{4}$$

where S denotes the surface area of the circular base of the cone, and z_c is the height of the cone surface above the area element dS, as shown in Fig. 4. The satellite altitude will be in excess of 200 km, so that the vertical extent of the plume is quite small compared to the height of the cone surface z_c, except near the intersection of the cone with the ground. Thus, the value of the integral in the z direction will not be changed significantly if the integration limit is extended from z_c to infinity. This simplification reduces the z integral to $(2\pi\sigma_z)^{1/2}$, and Eq. (4) becomes

$$P=\frac{KQ}{(2\pi)^{1/2}u}\int\int_S \frac{1}{\sigma_y}\exp[-1/2(\frac{y}{\sigma_y})^2]dS \tag{5}$$

where (see Fig. 3): $\sigma_y=c_y x; X=(X-X_s)\cos\theta+(Y-Y_s)\sin\theta;\ y=-(X-X_s)\sin\theta+(Y-Y_s)\cos\theta$; and $S=\{X,Y: (X-X_m)^2+(Y-Y_m)^2\leq R^2\}$. It is seen that the measurement is independent of σ_z and H.

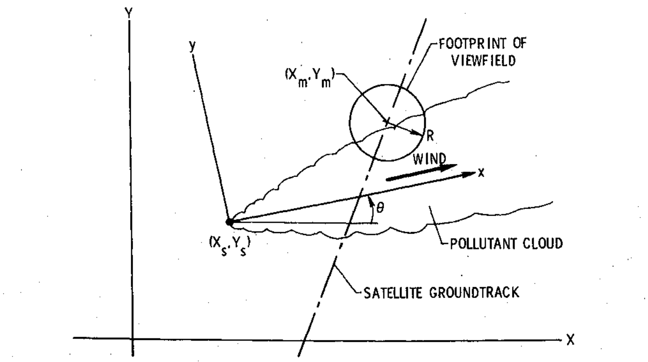

Fig. 3 Coordinate systems used in computing pollution concentrations.

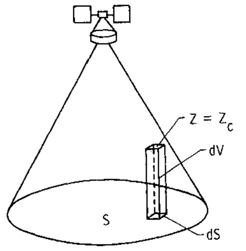

Fig. 4 Volume integral within cone of viewing field.

Parameter Estimation

The estimation procedure which will be used in this paper is a weighted least-squares fit of computed measurements to the observed measurements.[6,7] From Eq. (5) it is seen that the computed measurement P may be expressed by use of the dispersal model as a function of the model parameters Q, u, c_y, θ, X_s, Y_s and the measurement location X_m, Y_m. The vector $\bar{x}$ is defined as the array of numbers (Q, u, c_y, θ, X_s, Y_s). The i^{th} computed measurement P_i may be expressed as

$$P_i=P(\bar{x};\ X_{m,i},\ Y_{m,i}) \tag{6}$$

Note that the model parameters c_z and H do not appear in Eq. (5), and thus are not listed as components of $\bar{x}$. In the present paper it will be assumed that the orbit is known exactly and that the satellite is oriented such that the instrument is pointed exactly along the nadir.

The problem may be stated at this point: given a set of observations Φ_i, what is the best estimate of $\bar{x}$? The "weighted least-squares batch processor" is used here. First, the function P_i is linearized about the best available estimate $\hat{x}$, where the caret denotes estimate. Then, the $\Delta\bar{x}=\bar{x}-\hat{x}$ which minimizes the weighted sum of the products of the residuals is determined. Thus, the residual is expressed as

$$\delta_i=\Phi_i-P_i(\bar{x})=\Phi_i-[P_i(\hat{x})$$
$$+\sum_{j=1}^{n}\frac{\partial P_i}{\partial x_j}\Big|_{\hat{x}}(\bar{x}_j-\hat{x}_j) \tag{7}$$
$$+\text{ higher order terms}]$$

where δ_i = residual of the i^{th} measurement, $\Phi_i = i^{\text{th}}$ observable measurement, $P_i = i^{\text{th}}$ computed measurement, and n = dimension of $\bar{x}$. In the present case, $n=6$. If there are m measurements, then

$$\begin{Bmatrix}\delta_1\\ \delta_2\\ \vdots\\ \delta_m\end{Bmatrix}=\begin{Bmatrix}\phi_1-P_1(\hat{x})\\ \phi_2-P_2(\hat{x})\\ \vdots\\ \phi_m-P_m(\hat{x})\end{Bmatrix}$$
$$-\begin{bmatrix}(\partial P_1/\partial x_1)\,(\partial P_1/\partial x_2)\cdots & (\partial P_1/\partial x_n)\\ (\partial P_2/\partial x_1)\,(\partial P_2/\partial x_2)\,\cdots & (\partial P_2/\partial x_n\\ \vdots\qquad\quad\vdots & \vdots\\ (\partial P_m/\partial x_1)\,(\partial P_m/\partial x_2)\quad\cdots & (\partial P_m/\partial x_n)\end{bmatrix}\begin{Bmatrix}\Delta x_1\\ \Delta x_2\\ \vdots\\ \Delta x_n\end{Bmatrix}$$

$$\bar{\delta}=\bar{\Phi}-\bar{P}(\hat{x})-\Lambda\,\Delta\bar{x} \tag{9}$$

It is emphasized that the measurements need not be taken by the same instrument, or of the same observable quantity. For example, the vector may include 15 data points from the satellite instrument and one measurement of wind speed. The weighted sum of squares of the residuals is then

$$S = \sum_{i=1}^{m} \sum_{j=1}^{m} W_{ij}\, \delta_i \delta_j = \delta^T W \delta$$

$$= (\bar{\Phi} - \bar{P}(\hat{x}) - \Lambda \Delta\hat{x})^T W (\bar{\Phi} - \bar{P}(\hat{x}) - \Lambda \Delta\hat{x}) \tag{10}$$

The necessary conditions that S be a minimum are

$\partial S/\partial x_l$ =

$$2 \sum_{i=1}^{m} \sum_{j=1}^{m} W_{ij} \Lambda_{il} (\Phi_j - P_j - \sum_{k=1}^{n} \Lambda_{jk} \Delta\hat{x}_k) = 0 \quad l \epsilon [1,n] \tag{11}$$

where

$$\Delta\hat{x} = (\Lambda^T W \Lambda)^{-1} \Lambda^T W (\bar{\Phi} - \bar{P}) \tag{12}$$

Equation (12) gives the correction which should be added to $\hat{x}$ to improve the estimate of $\bar{x}$, and is known as the weighted least-squares batch processor. Equation (12) is applied iteratively until $\hat{x}$ converges, that is, $\Delta\hat{x}$ becomes sufficiently small. It is seen that for $\Delta\hat{x}$ to be uniquely defined, $(\Lambda^T W \Lambda)^{-1}$ must exist. This requirement is called the observability condition.[6] Note that if c_z had been included in $\bar{x}$, Λ would have a column of zeros for $\partial P_i/\partial c_z$, which would result in $\Lambda^T W \Lambda$ being singular, and $\Delta\hat{x}$ being undefined. Thus, the method would indicate that because the measurement is not influenced by c_z, then c_z cannot be inferred from the measurements. The inverse of the covariance matrix of the data is used for weighting of the residuals. For a linear process with normally distributed errors, this estimate provides a minimum variance, maximum likelihood unbiased estimate of the true parameters.[6] Throughout the remainder of this paper, the weighting matrix W will be the inverse of the covariance matrix of the data. The effect of this is to put a large weighting on highly accurate measurements and a small weighting on measurements which are not accurate.

Because of random variations in the measurements, $\bar{\Phi}$ is a random vector, thus, by Eq. (12) $\Delta\hat{x}$ is a random vector also. The covariance matrix for $\Delta\hat{x}$ is defined by

$$\text{cov}(\Delta\hat{x}) = E[(\Delta\hat{x} - E(\Delta\hat{x}))(\Delta\hat{x} - E(\Delta\hat{x}))^T] \tag{13}$$

and is a measure of how well $\Delta\hat{x}$ is known. By use of Eq. (12) it can be shown that

$$\text{cov}(\Delta\hat{x}) = (\Lambda^T W \Lambda)^{-1} \tag{14}$$

where now

$$W = [\text{cov}(\bar{\Phi})]^{-1}$$

Thus, the observability condition may be stated in terms of the existence of cov $(\Delta\hat{x})$. The matrix

$$M = \Lambda^T W \Lambda$$

is called the information matrix. The application of parameter estimation techniques for the interpretation of satellite pollution data will now be considered.

Application and Results

To interpret satellite pollution data, it is necessary, as will be shown, to use additional data types. Thus, the instrument output as expressed in Eq. (5) will give a number of data points, which will be supported by other measurements; for example, of wind speed.

Central to the parameter estimation procedures is the matrix of partial derivatives, $\Lambda = [\partial P_i/\partial x_j]$, in which there is a row for each data point and a column for each parameter. It is assumed in this paper that the satellite orbit is known exactly and the instrument is pointed exactly, so that the region over which the integration is carried out is known. The partial derivatives of the computed output are thus given by

$$(\partial P_i/\partial Q) = (P_i/Q) \tag{15a}$$

$$(\partial P_i/\partial u) = -(P_i/u) \tag{15b}$$

$$\frac{\partial P_i}{\partial c_y} = -\frac{P_i}{c_y} + \frac{Q}{(2\pi)^{1/2} u c_y^4} \times \int\int_{S_i} \frac{y^2}{x^3} \exp\{-\frac{y^2}{2c_y^2 x^2}\} dS \tag{15c}$$

$$\frac{\partial P_i}{\partial \theta} = \frac{Q}{(2\pi)^{1/2} u c_y} \int\int_{S_i} \frac{y}{x^2} [\frac{x^2+y^2}{c_y^2 x^2} - 1] \times \exp\{-\frac{y^2}{2c_y^2 x^2}\} dS \tag{15d}$$

$$\frac{\partial P_i}{\partial X_s} = \frac{Q}{(2\pi)^{1/2} c_y} \int\int_{S_i} \frac{1}{x^2} [\cos\theta - \frac{y(x\sin\theta + y\cos\theta)}{c_y^2 x^2}] \times \exp\{-\frac{y^2}{2c_y^2 x^2}\} dS \tag{15e}$$

$$\frac{\partial P_i}{\partial Y_s} = \frac{Q}{(2\pi)^{1/2} u c_y} \int\int_{S_i} \frac{1}{x^2} [\sin\theta + \frac{y(x\cos\theta - y\sin\theta)}{c_y^2 x^2}] \exp\{-\frac{y^2}{2c_y^2 x^2}\} dS \tag{15f}$$

To compute P_i and the elements of Λ, it is necessary to perform an integration over a circle. A technique for conveniently doing this is presented in Ref. 8.

Examination of Eqs. (15a) and (15b) shows that the first and second columns of the Λ matrix are linearly dependent, that is

$$(\partial P_i/\partial Q) = -(u/Q)\ (\partial P_i/\partial u) \tag{16}$$

where $(-u/Q)$ is a constant for all rows in the Λ matrix. It then follows that the information matrix M is singular, so that its inverse, the cov $(\Delta\hat{x})$ matrix does not exist and the system is not observable. It is seen that Q and u may be varied such that Q/u remains constant without changing the pollutant concentration field. A separate measurement is needed to determine Q and u separately. The Q and u will be replaced by a single variable Q/u, and Eqs. (15a) and (15b) are replaced by

$$(\partial P_i/\partial(Q/u)) = (P_i/Q/u)$$

A numerical example will now be considered.

Numerical Example

The following nominal condition will be considered. The source will be assumed to be at the origin of the earth-fixed coordinate system, and the wind blowing along the X-axis. The satellite ground track will be parallel to the Y-axis along the line $X = 90$ km. The radius of the instrument footprint (the base of the conical view field) is 30 km. The instrument output constant K and Q/u are assumed to be unity, and c_y is assumed to be 0.1. In each case, there is a data point at $Y = -150$ km, with additional points at regular intervals up to $Y = 150$ km.

For the present study, the most convenient measure of data rate is the distance between data points, that is, the distance between the centers of the successive circular footprints. The distance between data points for a satellite in a circular orbit at various altitudes is shown as a function of data rates in Fig. 5.

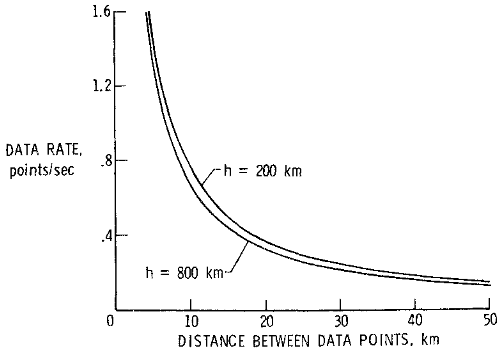

Fig. 5 Data rates as a function of distance between data points for satellites in circular orbits at 200 and 800 km altitude.

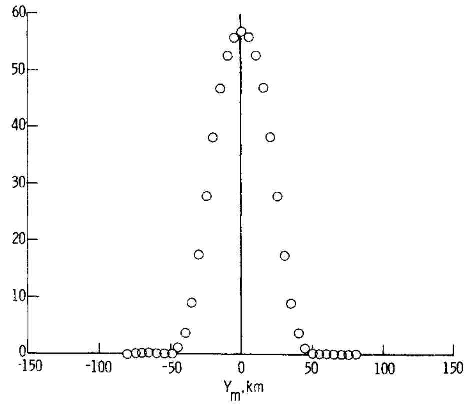

Fig. 6 Instrument output as a function of measurement station. Ground track 90 km downwind of source.

Table 1 Additional data types assumed

Case	σ_{c_y}	σ_θ	σ_{X_s}	σ_{Y_s}
1	...	...	...	...
2	0.1	...	...	...
3	...	0.1	...	...
4	...	...	1.0	1.0
5	...	...	1.0	1.0
6	0.1	...	1.0	1.0
7	...	0.1	1.0	1.0
8	0.1	0.1	1.0	1.0

The instrument output is shown in Fig. 6 for a data rate corresponding to 5 km between data points. In addition to the satellite data, there may be a measurement of the wind direction θ, an estimate of the dispersion parameter c_y based on atmospheric conditions (including wind speed and insolation) or an estimate of the source location X_s, Y_s. These additional data types will each have associated errors. Various combinations of these with the satellite data are considered, with standard deviations listed in Table 1. The dotted lines in Table 1 indicate that the data are assumed to be unavailable. It is pointed out that the standard deviation of the estimate of a given parameter based on all available data will be smaller than the standard deviation of the estimate of that parameter based on a single data type. It is assumed that the standard deviation of the instrument error ϵ is one. The standard deviations of the parameters are shown in Figs. 7-11 as a function of the distance between data points for Cases 1-8.

Using satellite data alone, that is, for Case 1, it is seen from Fig. 7 that the wind weighted source strength Q/u may be determined accurately for a distance between data points up to 20 km. For 30 km spacing the accuracy is so poor ($\sigma_{Q/u} = 12$) that the point is outside the range of the figure. For data points 40 km or farther apart, the standard deviations are so large that the information matrix is ill conditioned and

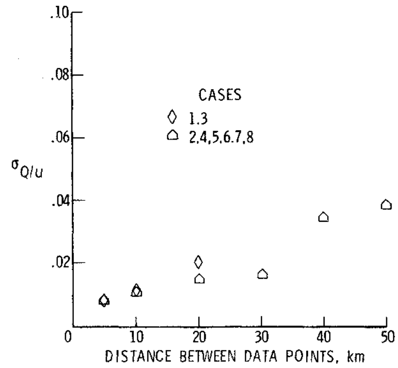

Fig. 7 Standard deviation of source strength divided by wind velocity as a function of distance between data points.

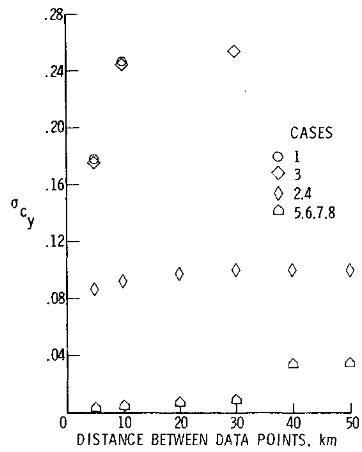

Fig. 8 Standard deviation of horizontal dispersion parameter as a function of distance between data points.

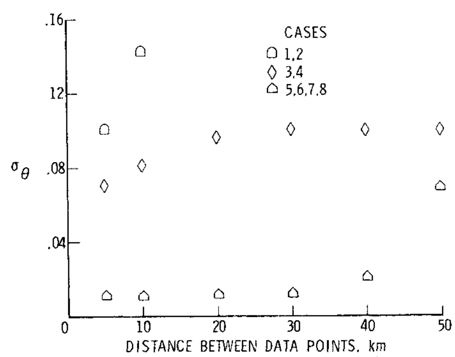

Fig. 9 Standard deviation of wind direction angle as a function of distance between data points.

the present technique must be considered to be useless for analyzing the data. However, if any additional information is available as in Cases 2-8, then Q/u may be determined fairly well.

The standard deviation of the dispersal parameter σ_{c_y} is plotted in Fig. 8 as a function of distance between data points. It is seen that satellite pollution data alone (Case 1) or with wind direction measurement (Case 3) will not provide a good estimate of c_y. However, given a good estimate of source location from other data types, the c_y may be estimated quite closely. Similar results are found for standard deviations of wind direction σ_θ, shown in Fig. 9. It is found that for data points 5 and 10 km apart, the wind direction may be determined with good accuracy ($\sigma_\theta \approx 6°$) using only satellite data (Case 1), but for 20 km or greater spacing the satellite data alone gives no information regarding wind direction. If an estimate of source location is available, the wind direction may be determined very accurately.

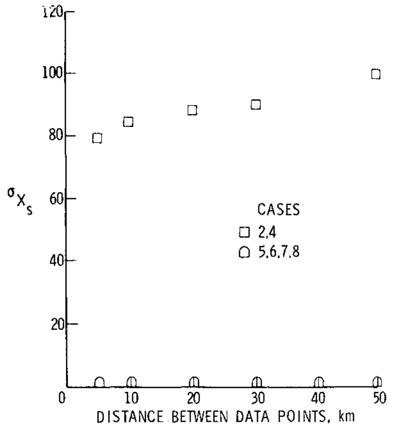

Fig. 10 Standard deviation of along-wind location of source as a function of distance between data points.

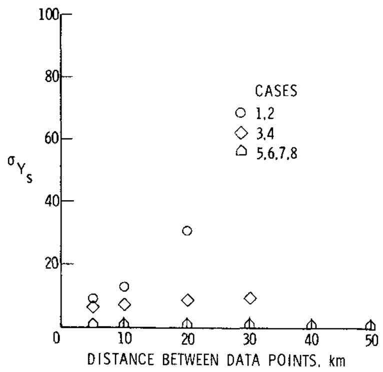

Fig. 11 Standard deviation of crosswind location of source as a function of distance between data points.

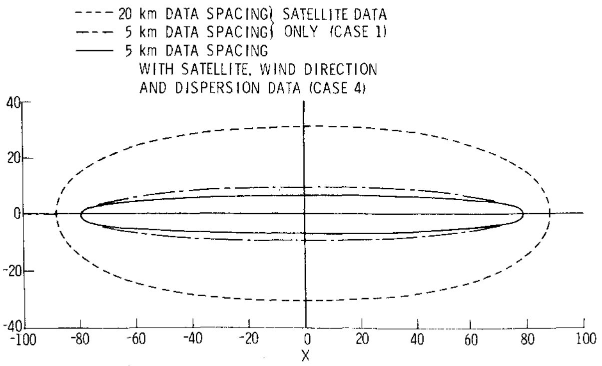

Fig. 12 One-sigma ellipses of source location for three conditions.

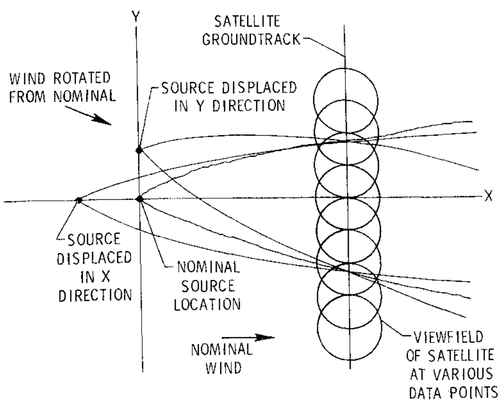

Fig. 13 Explanation of correlation between θ and Y_s and between c_y and X_s.

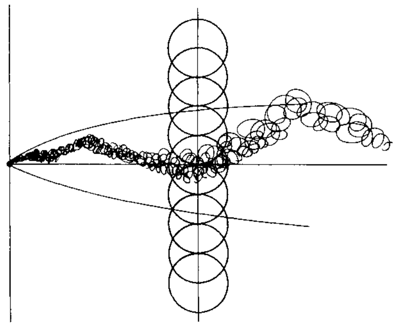

Fig. 14 Comparison of estimation problem for simple Gaussian plume and meandering plume.

The standard deviations of the estimate of the source location, σ_{X_s} and σ_{Y_s}, are shown in Figs. 10 and 11 as functions of distance between data points. Without another data type providing an estimate of the dispersal parameter c_y, σ_{X_s} is rather large. Given an estimate of c_y (Cases 2 and 4), it is seen that σ_{X_s} is on the order of 80 km. Likewise, Fig. 11 shows that for 20 km or more between data points, an estimate of wind direction θ is quite helpful in reducing σ_{Y_s}. Using the results shown in Figs. 10 and 11 and assuming a gaussian distribution, probability of location ellipses may be drawn in Fig. 12. Shown there for three conditions are "one-σ ellipses," that is, ellipses whose major and minor axes are σ_{X_s} and σ_{Y_s}, respectively. Because the satellite ground track is parallel to the Y-axis, and the wind is parallel to the X-axis, the axes of the ellipse are aligned with the coordinate axes. Along the boundary of the ellipse, the probability density of the location of the source is a constant, and the probability density is greater within the ellipses. The probability of the source being within a one-σ ellipse is 0.394. If one were attempting to locate the source, this would be the prime search area.

The correlation matrix, defined by

$$\rho_{ij} = \text{cov}(\Delta\hat{x})_{ij} / \sigma_i \sigma_j$$

shows a high correlation between θ and Y_s and between c_y and X_s. Physically, the problem may be viewed as follows: consider the source to be displaced in the Y direction and the wind direction θ to be changed from the nominal as sketched in Fig. 13. Then the pollution burden in the view field and the output from the satellite will be changed only slightly. This results in a dependency between Y_s and θ and difficulty in separating the variations of these two parameters. Likewise, if the source is displaced upwind (that is, along the $-x$ axis) and the c_y decreased from the nominal value, then the pollution burden as viewed by the satellite will be changed only slightly.

Discussion

Linear parameter estimation theory is used with a simple pollution dispersal model (Gaussian plume) to provide a method for estimating the parameters and pollution concentration field and for computing the accuracy of these estimates. Study of a numerical example gives considerable insight into the process; nevertheless, results obtained from a single example are necessarily narrow.

One very interesting question raised by the present paper is how would the analysis be affected by replacing the deterministic plume model by a more realistic model? Once the parameters of the model have been specified, the plume is fixed and the instrument signal contains enough information that values for all five of the parameters can be extracted. In the real case, the vagaries of the atmosphere cause the plume to fluctuate randomly, as depicted in Fig. 14. This randomness must result in a loss of information in the plume, and at present, it is a moot point whether or not all of the parameters can be estimated from satellite data alone. A study using a stochastically meandering plume should be of use in resolving this question, though considerably more difficult.

The theory used here provides a solution which gives a local minimum to the weighted sum of squares of residuals. The question of uniqueness and selection of the solution in the event of multiple solutions arises. For example, in the present problem using satellite data only, an equally good solution for the data would be given by changing the wind direction 180° and putting the source at $X = 180$ km, $Y = 0$ instead of at the origin. In practice, other information would resolve this ambiguity, but the choice may not always be obvious. A problem with the linearized theory is seen in Fig. 12. Although the probability that the wind has a negative component along the X-axis is vanishingly small for Case 4, a two-sigma ellipse would have a large portion of its area downwind of the satellite ground track, corresponding to a significant probability that the source is downwind of the ground track. This is simply an indication that for the numbers assumed for this example a distance of one standard deviation along the X-axis is beyond the linear range. It may be necessary to develop a theory which is nonlinear in at least the X_s variance. Finally, it was noted that in some cases, the information matrix was ill conditioned. For these cases, the data rate was simply inadequate. However, it may be possible to obtain some results from such data using other approaches.

In Figs. 8 and 10, it is found that more information was obtained by data at 50 km intervals than by data at 40 km intervals. This is because the few 50-km data points happened to be positioned better relative to the plume than the few 40-km data points. A translation of the source in the Y direction a few kilometers could reverse this.

In the present paper, an inert pollutant was assumed. A model could be used which includes chemical reactions and scavenging processes. An interesting extension of the present work would be to study these processes through the parameter estimation procedures. For example, a reaction rate constant could be included in the parameter vector to be estimated. In this regard, it must be emphasized that in the present application the procedures give a weighted least-squares fit to the model. If the model only grossly matches the situation, the results will be gross also.

Conclusions

Parameter estimation theory is used with a Gaussian plume model to provide a method for estimating the parameters and pollution concentration field and for computing the accuracy of these estimates. From this study the following conclusions are made: 1) Measurements of the total mass of an air pollution species within a volume determine source strength Q divided by wind velocity u, (Q/u). In order to estimate Q, a measurement of u is required. 2) Errors in the wind direction estimate are highly correlated with errors in the crosswind distance of the source location estimate. 3) Errors in the horizontal dispersion estimate are highly correlated with errors in the upwind distance estimate of the source location. 4) Errors in the upwind distance estimates of the source location are much larger than crosswind estimates of source location, even for high data rates. A possible extension of the study is to consider chemical reactions and scavenging processes and also to study the effect of the stochastic nature of the plume dispersal in the atmosphere on the estimation problem.

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