A Method to Determine the Spatial Resolution Required to Observe Air Quality From Space

Christopher P. Loughner, David J. Lary, Lynn C. Sparling, Ronald C. Cohen, Phil DeCola, and W. R. Stockwell

***Abstract*—Satellite observations have the potential to provide an accurate picture of atmospheric chemistry and air quality on a variety of spatial and temporal scales. A key consideration in the design of new instruments is the spatial resolution required to effectively monitor air quality from space. In this paper, variograms have been used to address this issue by calculating the horizontal length scales of ozone within the boundary layer and free troposphere using both *in situ* aircraft data from five different NASA aircraft campaigns and simulations with an air-quality model. For both the observations and the model, the smallest scale features were found in the boundary layer, with a characteristic scale of about 50 km which increased to greater than 150 km above the boundary layer. The length scale changes with altitude. It is shown that similar length scales are derived based on a totally independent approach using constituent lifetimes and typical wind speeds. To date, the spaceborne observations of tropospheric constituents have been from several instruments including TOMS, GOME, MOPITT, TES, and OMI which, in general, have different weighting functions that need to be considered, and none really measures at the surface. A further complication is that most satellite measurements (such as those of OMI and GOME) are of the vertically integrated column. In this paper, the length scales in the column measurements were also of the order of 50 km. To adequately resolve the 50-km features, a horizontal resolution of at least 10 km would be desirable.**

***Index Terms*—Air-quality observations, length scales, variograms.**

I. Introduction

IT IS CONCEIVABLE that many different criteria could be used to determine the spatial resolution needed to observe air quality from space, for example, the ability to resolve the finest structures in the trace gas fields (for aerosols or NO_2, this would be on the level of individual streets in a city) or the ability to resolve the typical structures in the air-quality fields. Since observing air quality at the scale of a few meters, necessary for street level monitoring, is likely to be beyond the reach of space observing systems, for a while, we would like to suggest a framework for objectively determining what the spatial scales of typical air-quality features are. To this end, this paper presents a variogramatic analysis which helps address the question, "what horizontal resolution is needed to observe air quality from space?" Since it is unlikely that there is a universal length scale applicable for all air-quality observations, it is useful to have a methodology for characterizing the spatial length scales needed for a given constituent under different conditions. We use this variogramatic approach for both *in situ* aircraft data from the five different NASA aircraft campaigns and regional model simulations at a range of resolutions.

A clear advantage of observing air quality from space is the global coverage which provides a broader context for source regions and allows transport away from the source regions to be monitored. However, what is not clear is the satellite spatial resolution required to quantitatively assess the relative impacts of individual sources.

As an example of applying a variogramatic approach for determining the required spatial resolutions for observing pollutants, we investigate the spatial distribution of tropospheric ozone in the polluted urban area of Los Angeles (LA) for early November. LA is an ideal choice for our study because its emissions are characterized, and it is a highly polluted urban area that is afflicted by both high levels of ozone and particulate pollution. Although ozone mixing ratios reach maximum levels during the summertime while concentrations of particulates maximize during the late fall and early winter, this paper is directed toward the use of satellites to observe air quality throughout the year. Also, one of the most important future applications of these observations will be to improve year-round air-quality forecasting. Accurate air-quality forecasts must include ozone at all concentrations and not just summertime peak values. As shall be seen, in the LA region, the length scales are rather short, at around 60–80 km in the atmospheric boundary layer. Tropospheric-ozone data from several global tropospheric experiment (GTE) missions suggest length scales from 50 to 150 km. In the eastern U.S., on the other hand, spatial correlations across ozone monitoring sites suggest longer scales of around 500–1000 km [1]–[3]. In contrast, for urban air-quality applications, air-quality models are typically used at resolutions down to 4 km to account for source variability.

The natural question to address is "what resolution do we need for satellite-borne observations of air quality?" Even though we do not conclusively answer this question, we can say that if the satellite measurements are to be useful, then they should be capable of capturing the spatial scales typically

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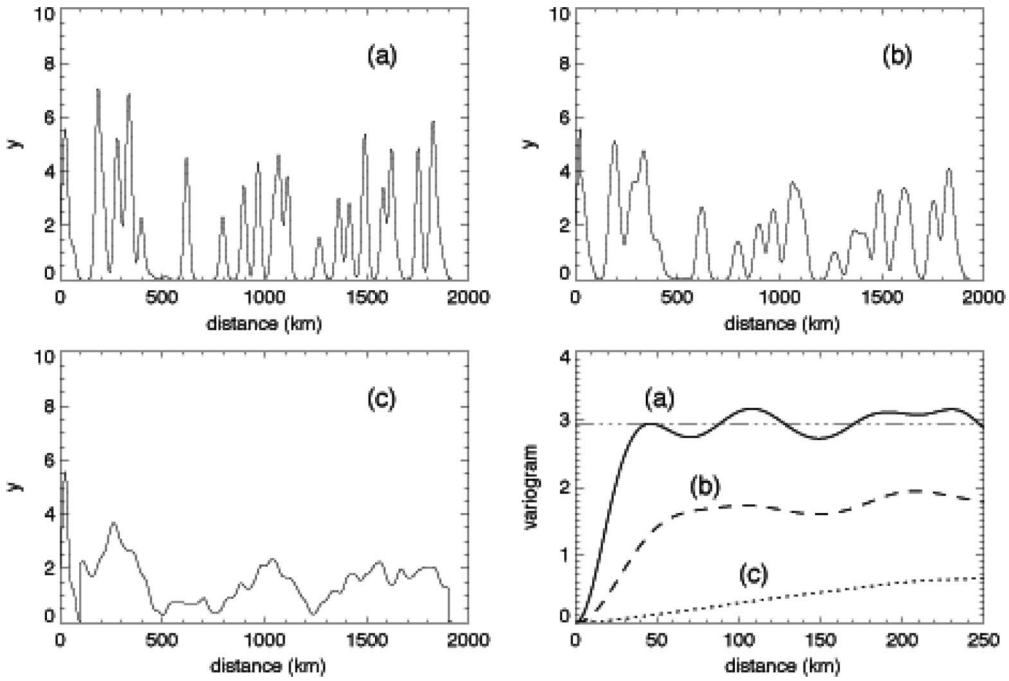

Fig. 1. Some examples of variograms constructed from a simulated 1-D datastream $y(x)$. (a) Data are composed of randomly placed structures with a characteristic scale of 40 km. (b) and (c) Boxcar-smoothed data, which are smoothed on scales of 50 and 200 km, respectively. The corresponding variograms are shown in the last panel. Case (a) shows damped oscillations due to the quasi periodicity; the first maximum occurs at the scale of the features, and the first minimum is on the order of the average separation between structures.

encountered, and we present a methodology for characterizing the length scale. We find that the spatial scales encountered are a strong function of altitude, and that the smallest scales are typically found in the planetary boundary layer and are of the order of 50–60 km. This is true in both the model and the observations. A methodology is presented that can be applied to both data and models that will provide some insight into spatial scales in air-quality fields which can be used to inform decisions about optimal satellite resolution. The following sections outline first the definition and use of variograms to determine length scales, and then the models and emissions inventory.

II. Variogram Analysis

A quantitative measure of the spatial variability of a field $y(\mathbf{x})$ can be obtained by sampling the field simultaneously at two points separated by a horizontal separation $\mathbf{h}$. The semivariogram is one-half the variance of the ensemble of field increments $y(\mathbf{x}_\mathrm{i}+\mathbf{h})-y(\mathbf{x}_\mathrm{i})$

$$\gamma(\mathbf{h})=\frac{\sum\left(y(\mathbf{x}_\mathrm{i}+\mathbf{h})-y(\mathbf{x}_\mathrm{i})\right)^2}{2N} \tag{1}$$

where N is the number of pairs with separation $\mathbf{h}$. The magnitude of the variance depends, in general, on both the magnitude and direction of the separation vector $\mathbf{h}$, sometimes called the "lag." A plot of variance as a function of distance or time is called a variogram. Variograms have been applied extensively in oil recovery and mining applications [4], and are being used more widely for characterizing atmospheric temporal and spatial variability such as the continuity of alpine precipitation [5]. Similar kinds of analyses have been applied to stratospheric chemical tracers [6] and cloud liquid water [7].

We should note that the variogram is essentially the physical space representation of the Fourier transform under conditions of statistical homogeneity. The variogram and Fourier transform are second-order measures of spatial variability, i.e., dependent on the square of the difference in the field between two points. Other scale-dependent measures of variability, such as the absolute deviation (the mean of the absolute value of the difference between two points) could also have been chosen; this gives the same results for the problem at hand, which is essentially to identify the correlation length. A further discussion of these points and an analysis of the probability density function of the increments can be found in [8].

To aid in interpreting the variograms from the model and data, some examples of variograms constructed from a simulated 1-D datastream $y(x)$ are shown in Fig. 1. In Fig. 1(a), the data are composed of randomly placed structures with a characteristic scale of 40 km. Fig. 1(b) and (c) shows the boxcar-smoothed data, which are smoothed on scales of 50 and 200 km, respectively. The corresponding variograms are shown in the last panel. Case (a) shows the damped oscillations due to the quasi-periodicity; the first maximum occurs at the scale of the features (40 km), and the first minimum at 70 km is on the order of the average separation between structures. This was inferred by constructing strictly the periodic structures with varying sizes and separations. Beyond the first minimum, $\gamma(h)$ oscillates about the dot-dashed line which is the variance of the data in Fig. 1(a).

Expanding the square, (1) can also be written as $\gamma(h)=\mathrm{var}(y) - <y(x+h)y(x)>$, where $\mathrm{var}(y)=\mathrm{var}(y(x))=\mathrm{var}(y(x+h))$ and $<y(x+h)y(x)>$ is the autocorrelation function. Thus, when h is larger than the correlation length h^*, $<y(x+h)y(x)>\approx 0$ and $\gamma(h)\approx\mathrm{var}(y)$. Smoothing over a

scale L, as in Fig. 1(b) and (c), induces a correlation length L which can be seen in the variograms of the smoothed data.

In variogram terminology, the scale corresponding to the first minimum or ledge is called the horizontal range [4].

In the case of the model simulations, ozone variograms were computed for each row (east–west direction) and each column (north–south direction), excluding the boundaries. These variograms were averaged to produce one east–west and one north–south variogram for all sigma levels and the total columns. Variograms were created using the Geostatistical Software Library [9] and analyzed for ozone from the comprehensive air-quality model with extensions (CAMx) model output run at various spatial resolutions. The ozone variograms were analyzed in order to characterize the scale-dependent variability of ozone throughout the lower troposphere in these two directions. A characteristic scale h^* was identified, as described below.

III. Model Simulations and Emissions Inventory

The air-quality modeling domain included the LA area. It was centered over LA with a horizontal range of 368 km east–west by 256 km north–south. MM5, a widely used mesoscale meteorology model [10], was used in this paper to provide the meteorological input for CAMx, a Eulerian photochemical dispersion model. MM5 is initialized with no locally thermally driven circulations. Therefore, model "spin up" is needed for the model to represent the atmosphere responding to mesoscale forcing from local features before CAMx is initialized. CAMx simulates emissions, dispersion, chemical reactions, and deposition of pollutants in the lower troposphere over urban and regional areas. The main features of the model are summarized below; details can be found in the CAMx User's Guide [11].

Within CAMx, pollution transports by advection and diffusion processes are solved using mass conservation and mass consistency approaches using equations in flux form. The continuity equation is operationally split to calculate separate contributions of emissions rates, horizontal advection, vertical advection, vertical and horizontal diffusion, wet scavenging, and chemistry at each time step within each grid cell in this order. Horizontal flux divergence of atmospheric density is calculated in a way that is numerically consistent with the horizontal transport of pollutants to ensure that there is mass consistency. Horizontal advection in CAMx is the area preserving flux-form advection [12], which is implemented according to the study in [13]. Horizontal eddy diffusion coefficients are calculated within CAMx based on the study in [14].

The vertical velocity profile at each time step is found by vertically integrating the divergent incompressible continuity equation, and gridded vertical diffusion coefficients are supplied to CAMx from MM5 output. Dry deposition velocities for each species are calculated based on the species' chemical properties, local meteorological conditions, and surface conditions. Dry deposition is used as the lower boundary condition for vertical diffusion, which is coupled with surface removal of pollutants through each column of cells by the vertical mixing process. Wet scavenging of gases and aerosols are calculated within CAMx, and the carbon bond mechanism version IV [15] is used to simulate the gas chemistry to complete the operator splitting approach of solving the continuity equation at each time step.

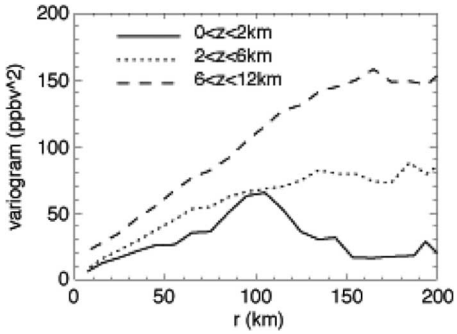

Fig. 2. Composite of five aircraft missions and how the variograms depend on altitude. The strong peak near 100 km is a robust feature seen in each mission.

Emissions used within the CAMx model for this paper are the National Center for Atmospheric Research (NCAR) Aeronomy Laboratory recompilation of the U.S. Environmental Protection Agency 1999 National Emission Inventory (NEI-99) version 3, which were obtained from the NCAR Aeronomy Laboratory (Stu McKeen, personal communication). The recompilation of this emission inventory was developed for the 2004 International Consortium for Atmospheric Research on Transport and Transformation/New England Air Quality Study regional forecast model intercomparison study. Emissions of NO_x, CO, SO_2, NH_3, PM10, 41 speciated VOC compounds, and five speciated PM2.5 aerosol components on an average summer day are included in the inventory. The gridded area emissions have a horizontal resolution of 4 km.

The MM5 horizontal grid was larger than the CAMx domain so that any artifacts which appeared at the MM5 horizontal boundaries were not passed to CAMx. There is always the possibility of artifacts (i.e., numerical noise) adjacent to the MM5 horizontal boundaries due to the boundary conditions coming into dynamic balance with MM5's algorithms. The vertical coordinates in the MM5 and CAMx model are terrain following or sigma coordinates. Twenty-nine sigma levels were used in the model ranging from the surface to 100 mb, and an ideal spatial resolution (the first maxima in the variogram) was found for the lowest five sigma levels, located within the boundary layer. For sigma level 1, the level closest to the ground, the pressure ranged from 1019 to 732 mb due to changes in elevation with a median pressure of 941 mb. Vertical soundings throughout the domain at low elevation sites (LA International, Catalina, and Long Beach Airports) showed a strong inversion from 975 to 925 mb.

MM5 and CAMx model runs were performed to simulate the state of the atmosphere in the LA basin and surrounding area for early November 2002 at 4-, 8-, 12-, and 16-km resolutions. The time period chosen for the modeling study corresponds to a field campaign made by the Desert Research Institute. The field campaign focused on aerosol formation which, for LA, tends to be greater during the late fall and early winter. The vertical resolution was kept the same with 29 sigma levels for all simulations. CAMx simulated the chemistry of the atmosphere

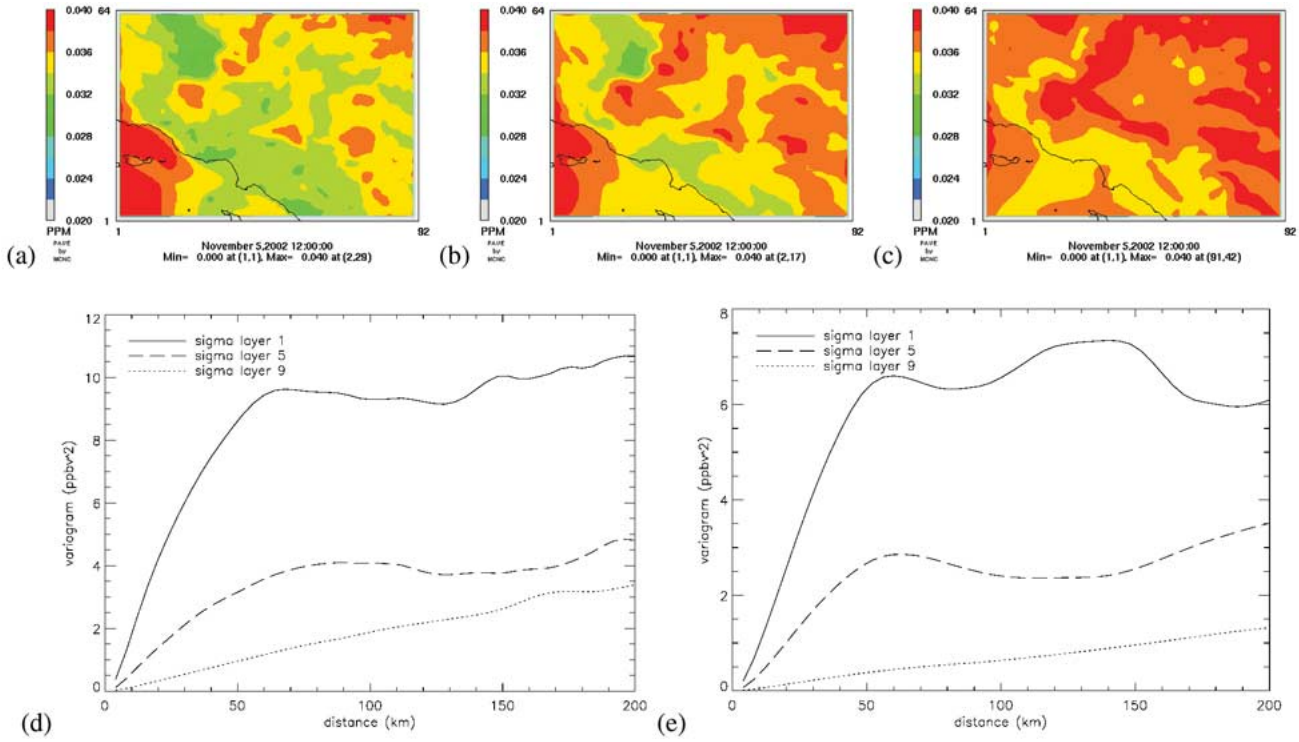

Fig. 3. (a) Contour plot of O_3 near the surface over the entire domain of the 4-km resolution model simulation for (a) sigma level 1 (sea level—2772 m, median = 685.5 m), (b) sigma level 5 (181.8–2892 m, median = 849.1 m), and (c) sigma level 9 (595.6–3248 m, median = 1253 m). In each case, the coast line is shown. (d) and (e) Corresponding ozone variograms with directional vector h from south to north and from west to east, respectively.

from 08 universal time (UT) on November 3 to 08 UTC on November 6. There was adequate "spin up" time for MM5, which ran from 00 UTC on October 31 through the CAMx simulations. Aircraft measurements were not available to provide aloft boundary conditions for LA during the period simulated. The aloft boundary conditions were provided by the model spin up, and this is a source of uncertainty in the simulations. Long-range transport toward the ocean, its return, and eventual subsidence are some of the sources of variability, but there is no apparent reason to believe that the resolution to observe these boundary effects would be any different than what is determined by this paper. In the future, satellite observations have the potential to provide the needed information on the long-range transport and eventual subsidence of air pollutants to air-quality models. The ozone field from the CAMx model at 20 UTC, November 5 was analyzed by the variogram method described below.

IV. Results and Discussion

A. Aircraft Data

Aircraft observations of ozone taken during several NASA GTE missions [Pacific Exploratory Missions (PEM) Tropics-A, B, PEM-West A, B, and Transport and Chemical Evolution over the Pacific—http://www-gte.larc.nasa.gov/] were combined and analyzed in order to investigate the altitude dependence of h^*. These missions were chosen because of the extensive sampling in the lower part of the atmosphere. Individual missions show qualitatively the same behavior as the composite. The horizontal scale characterized by the variogram does change with altitude as can be seen from the aircraft ozone variograms shown in Fig. 2. This figure shows how the horizontal scale depends on altitude and, therefore, that the required solution for a satellite will depend on the observed vertical level.

B. Air-Quality Simulations

By way of comparison, Fig. 3(a)–(c) shows the ozone concentrations in the entire model domain at 2000 UTC November 5, noon local time, for sigma levels 1, 5, and 9 with a 4-km resolution. The corresponding variograms are shown in Fig. 3(d) and (e), with directional vector $\mathbf{h}$ from west to east and south to north, respectively.

The ozone field shows a quasi-periodic spatial structure [Fig. 3(a)–(c)], and the variograms [Fig. 3(d) and (e)] show behavior similar to that shown in Fig. 1. The model was run at spatial resolutions of 4, 8, 12, and 16 km to see if there was any dependence of the horizontal range h^* (the correlation length) on the model resolution. The horizontal range converged to a well-defined spatial resolution of approximately 60 km in the boundary layer [Fig. 3(d) and (e)]. Remote near-surface ozone monitoring—if possible—would have to resolve features on the order of 60 km to capture the dominant scales in the ozone field in this example. With the increasing altitude, h^* increases and, at the top of the boundary layer, exceeds the model grid scale of 200 km. The horizontal ozone gradient is strongest near the surface, and variograms of the tropospheric ozone column (not shown) resemble the variograms of the lowest model layers. We note that there is some anisotropy between the north/south and east/west length scales, which is probably due to wind direction and topography.

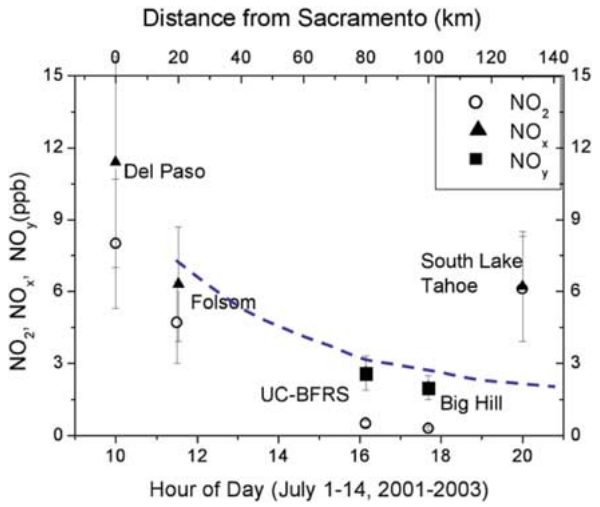

Fig. 4. Concentrations of nitrogen species as a function of their distance from Sacramento (upper x axis) [16]–[18].

The comparison between the model and observations is complicated as the model sigma level 1 focuses exclusively on the boundary layer, and it is not practical to have an aircraft fly over LA at an altitude of 50 m. Therefore, generally, we have more limited aircraft data in the boundary layer. However, we see in the 0- to 2-km-altitude curve of Fig. 2 a ledge at around 50 km that closely corresponds to the model's length scale of 60 km. The main length scale picked up in the five aircraft campaigns considered was 100 km. This increased to around 140 km for 2- to 6-km-altitude case and 160 km for 6- to 12-km-altitude case.

The variogram analysis for the total tropospheric column obtained a spatial length scale of 60 km, reflecting the near surface ozone spatial scale.

C. Other Estimates of Spatial Scales

As a sanity check, it is useful to look at other estimates of the spatial scales involved with air quality. Another way to estimate the spatial scales that an air-quality satellite would need to resolve is to use constituent lifetimes. For example, NO_2 has a chemical lifetime of approximately 6 h. Therefore, in 6 h with a typical wind speed of 3 $\mathrm{m} \cdot \mathrm{s}^{-1}$, air moves around 60 km. This is consistent with the results of other studies [19], [20]. Therefore, if we are to observe that spatial change in NO_2 from space, we need a resolution well below 60 km.

A length scale of around 60 km is also shown in Fig. 4, which shows the concentrations of various nitrogen species as a function of their distance from Sacramento [16]–[18].

The region from Sacramento to Lake Tahoe has an extremely regular meteorology with a typical mountain–valley flow pattern. In the daytime, westerlies move air from Sacramento to the upslope. The transport pattern results in the arrival of a plume originating in the city of Sacramento, CA, 50-km upwind at the University of California–Blodgett Forest Research Station (UC-BFRS), and at the Big Hill sites almost every day with little variation in transit time. As a consequence of this regularity, all of the observations we present are from a single source region. The approximate exponential decay observed reflects both chemical conversion of NO_x to higher oxides and dilution of the urban plume into the regional background. We note that the NO_x concentration at 120 km from Sacramento is approximately half of that at 60 km from Sacramento (i.e., an e-folding length scale of approximately 60 km). Likewise, NO_x falls by slightly more than 1/e between Folsom and UC-BFRS, indicating an e-folding length scale of just under 40 km between these two sites.

V. Conclusion

The variogram analysis discussed here offers a potentially useful way of determining the minimum spatial resolution required for satellite monitoring of air-quality fields, namely, by matching the satellite resolution to the characteristic scales of variability seen in atmospheric constituents that are important for air quality. For satellite observations of the air-quality fields to be useful in examining issues such as source assignment, etc., the observations need to be able to resolve the smallest length scales in the air-quality fields of constituents such as ozone. In this paper, we found that the smallest length scales were present in the boundary layer and were of the order of 60 km in the model and 50 km in the data. To adequately resolve the air-quality fields with length scales near 60 km, it would be desirable to have at least a 15-km resolution for the satellite observations.

MM5 and CAMx simulations were performed at resolutions of 4, 8, 12, and 16 km. Ozone-concentration results in the lower troposphere from the CAMx simulation were used to produce variograms in order to identify the length scales of ozone variability in the lower troposphere. The small-scale correlation length h^* for the variability in N–S and E–W directions was identified.

The model length scales calculated depend on the model's description of mixing in the boundary layer and the free troposphere. A multimodel study is underway to examine this issue. It should also be noted that we tried to calculate the length scales throughout the troposphere, but unfortunately, the model domain was smaller than the spatial length scale, so h^* could not be found. To date, the spaceborne observations of tropospheric constituents have been from several instruments including TOMS, GOME, MOPITT, TES, and OMI which, in general, have different weighting functions that need to be considered, and none really measures at the surface. A further complication is that most satellite measurements (such as those of OMI and GOME) are of the vertically integrated column. In this paper, the length scales in the column measurements were also of the order of 60 km. A good description of this issue for the case of MOPITT is given by [21].

Although this model analysis was for a limited set of conditions in the LA Basin, it is a representative of the kinds of areas of interest for air-quality monitoring. Although some might assume that the variability in ozone concentrations is greater during its summertime maxima, this may not be true. Given that the seasonal variability of nitric oxide emission rates is low in LA, the overall lower ozone concentrations during the late fall and winter months could show greater variability due to a greater proportional effect of nitric oxide titration on ozone

mixing ratios. For a satellite platform to effectively monitor the air quality, it should have a spatial resolution sufficient to fully resolve the length scale characterized by the first maximum of the variogram, and preferably, it should be lower. The length scales typically increase with altitude, so the required satellite resolution will depend on the observed vertical level. To fully assess how h^* varies within the boundary layer, a large database of boundary layer data would be required.

Sources have immediate influence on spatial scales of less than 1 km, so if one wanted to directly observe the NO_2 from a highway or to separate a particular factory/power plant from its surrounds, we would need another order of magnitude improvement over the 10–15 km we suggest.

Scale-dependent statistical methods, such as the variograms used here, might be useful in air-quality analyses which combine information with different spatial resolution such as surface data, satellite data, and models. If this paper were extended to consider temporal resolution as well, that could be of use for evaluating the relative merits of using geostationary satellite (GEO), Lagrange point (L1), or low Earth orbit satellites for air-quality applications. In this paper, we have concentrated exclusively on how variograms can be used to characterize the scales of horizontal spatial variability. However, a further complication beyond the scope of this paper is that most satellite measurements (such as those of OMI and GOME) are of the vertically integrated column. It is clear, however, that to the extent that satellite measurements average over horizontal and vertical variability to different degrees, it is necessary to understand the vertical and horizontal variability separately [8].

The examples considered here are not exhaustive but do demonstrate the utility of variograms for discussing the issue of required satellite resolution for observing air-quality. In order to fully address this issue requires more extensive investigation under a variety of conditions. In particular, spatial variability at the smaller scales may also be sensitive to model assumptions related to mixing and dispersion processes, and a study of these aspects of air-quality modeling is underway. We note that a realistic representation of scale-dependent variability will depend to some extent on the model dispersion.

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W. R. Stockwell, photograph and biography not available at the time of publication.