Generating High Spatial Resolution Analyses of SBUV Stratospheric Ozone for Calculating the Tropospheric Ozone Residual (TOR)

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Abstract- In the last decade, daily analyses of the Tropospheric Ozone Residual (TOR), which is an estimate of the vertically-integrated ozone in the troposphere, has been calculated as the difference between the vertically-integrated stratospheric ozone using data from the Solar Backscatter Ultraviolet (SBUV) remote sensing system and the total ozone from the Total Ozone Mapping Spectrometer (TOMS). Comparison of daily values of the TOMS/SBUV TOR with daily values of the surface ozone concentration and of the vertically-integrated ozone in the troposphere using ozonesonde data provided poor correlations. Reasonably good correlations were noted for longer-term (monthly, seasonally, and annually) averaged data. One of the major problems in applying SBUV data with TOMS data to develop daily estimates of the TOR is the difference in the spatial resolution. The SBUV instrument is a non-scanning, downward-looking radiometer. Data are only collected with 200-km spatial resolution along the orbital track of the satellite on which the instrument resides. The orbital tracks are as much as 25° longitude apart. The TOMS total ozone data, on the other hand, are collected globally on a daily basis at 50 km spatial resolution. The SBUV data gaps have been traditionally filled using conventional interpolation procedures so that the stratospheric ozone from the SBUV instrument would be available at the data locations of the TOMS instrument. Conventional interpolation procedures that have been used to fill the SBUV data gaps [e.g., linear and higher order spatial regression, kriging, basis functions, neural networks] have lacked the scientific methodology to include rigorously essential sources of physical knowledge and the conceptual organization to account for composite space-time variability effects; and, therefore, lack the ability to account for features that may exist between SBUV data sampling tracks. This factor is a cause of major errors found in the daily values of the TOMS/SBUV TOR. The objective of this study is to find an interpolation procedure that will provide significantly improved analyses of SBUV stratospheric ozone in the regions defined by the SBUV data gaps than is presently be acquired using conventional interpolations procedures. For this study, the Bayesian Maximum Entropy (BME) interpolation procedure of Modern Spatiotemporal Geostatistics was used to integrate efficiently salient physical knowledge about ozone in order to generate realistic analyses of ozone distribution across space and time. In addition to the satellite ozone measurements, BME interpolation procedure used secondary (soft) information such as the total ozone-tropopause pressure empirical relationship. The results suggested that BME interpolation procedure could eliminate a major source of error in the TOMS/SBUV TOR analyses (i.e., interpolation error), producing high spatial resolution analyses that are more accurate and informative than those presently produced using conventional interpolation techniques.

1. INTRODUCTION

Analyses of total ozone have been produced on a global basis using data from the Total Ozone Mapping Spectrometer (TOMS) since the late 1970s. In the last decade, climatological analyses of the Tropospheric Ozone Residual (TOR), which is an estimate of the total tropospheric ozone and which was, in the initial work, the difference between the total ozone from TOMS and the stratospheric ozone determined from the Stratospheric Aerosol and Gas Experiment (SAGE) instrument, have been developed [1, 2]. TOMS total ozone data are collected globally on a daily basis at 50 km spatial resolution, but the integration of years of SAGE data were required to provide a reliable analysis of the stratospheric ozone on a global basis because SAGE provided a very limited number of observations on any given day [3]. Subsequently, attempts have been made to develop daily maps of the TOR using data from the Solar Backscatter Ultraviolet (SBUV) remote sensing system, which are used to establish values for the stratospheric ozone on a daily basis [4]. However, direct comparison of variations of daily values of the TOMS/SBUV TOR with the variation of the daily values of the surface ozone concentration and of the vertically-integrated ozone in the troposphere using ozonesonde data provided poor correlations [3,5]. Reasonably good correlations were noted between longer-term (monthly, seasonally and annual), average TOMS/SBUV TOR values and surface ozone concentrations, as well as between climatological TOMS/SBUV TOR and ozonesonde data [1,3,5,6,7]

One of the major problems in applying SBUV data with TOMS data to develop estimates of the TOR is the difference in the spatial resolution. The SBUV instrument is a non-scanning, downward-looking radiometer. Data are only collected with 200-km spatial resolution along the orbital track of the satellite on which the instrument resides. For illustration purposes, the locations of TOMS total ozone measurements obtained on 6 July 1988 are shown in Fig. 1 (i.e., the small crosses). Triangles in Fig. 1 indicate the locations of the SBUV measurements on the same day. Clearly, TOMS provides more complete coverage because of its ability to scan while the satellite moves along the orbital track, whereas large SBUV data gaps exist between orbital tracks.

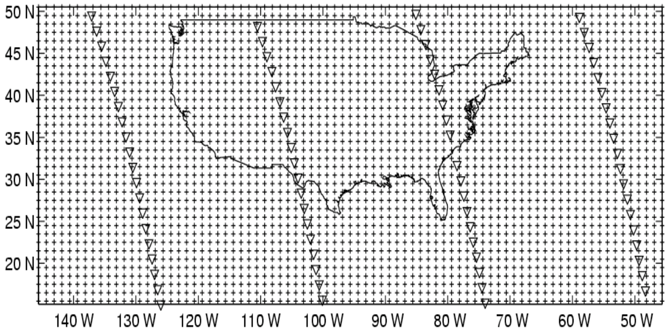

Fig 1 Location of satellite ozone observations on 6 July 1988 for TOMS (plus markers) and SBUV (triangles) instruments.

The SBUV data gaps have been traditionally filled using conventional interpolation procedures so that stratospheric ozone from the SBUV instrument would be available at the data locations of the TOMS instrument. Fig. 2 shows a comparison of stratospheric ozone from the SBUV instrument with the stratospheric ozone derived as the difference between the TOMS total ozone and the tropospheric ozone from the Wallops Island ozonesonde data. The comparison is made only on days when actual SBUV and TOMS measured values, not an interpolated data point, were located at the Wallops Island site in the period 1985-1989 (i.e., stratospheric ozone values were based entirely on measured data). In this case, the stratospheric ozone values from the SBUV instrument are well correlated with the stratospheric ozone derived from the TOMS total ozone and ozonesonde data. Fig. 3, on the other hand, provides a comparison between stratospheric ozone from the SBUV instrument with the stratospheric ozone from the TOMS and ozonesonde data when only interpolated SBUV

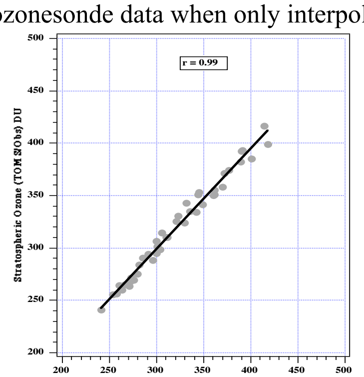

Figure 2 The stratospheric ozone (Dobson Unite-DU) derived using TOMS and the Wallops Island ozonesonde versus the stratospheric ozone from the SBUV using matched TOMS and SBUV at the Wallops Island location for the period 1985-1989.

data were used. The poor correlation between the two data sets demonstrates the problem with using conventional interpolation procedures to fill the data gaps between orbital tracks.

2. BME INTERPOLATION PROCEEDURE

Conventional interpolation procedures (e.g., linear and higher order spatial regression, kriging, basis functions, neural networks), which have been used to fill the SBUV data gaps, lack the scientific methodology to include rigorously essential sources of physical knowledge and also

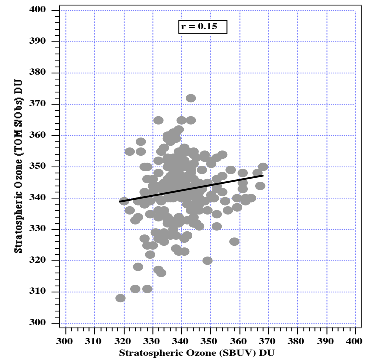

Figure 3 The stratospheric ozone derived using TOMS and the Wallops Island ozonesonde versus the stratospheric ozone from the SBUV using only interpolated *SBUV* data at the Wallops Island location for the period 1985-1989.

lack the conceptual organization to account for composite space-time variability effects. On the other hand, the Bayesian Maximum Entropy (BME) theory [8, 9] does not make any of the restrictive assumptions of conventional interpolation techniques mentioned above. BME gives high priority to a knowledge synthesis system that combines principles of rational reasoning with empirical evidence to improve the interpolation of ozone representation across space-time. For more details of the theory and mathematics associated with the BME interpolation procedure, see Ref [9]

For this study, the distribution of total ozone over the continental U.S.A. on July 6, 1988 was examined as an initial test of the BME interpolation procedure. TOMS total ozone data at the locations closest to the SBUV sampling points were selected for the analysis instead of SBUV stratospheric ozone data because a) the differences in the level of accuracy between the SBUV and TOMS instruments need not be accounted for in the analysis procedure and b) data to test the accuracy of the interpolated data was readily available for the entire domain using all available TOMS data. The BME interpolation procedure used an empirical relationship between tropopause pressure and total ozone, which was critical in accounting for the variability of ozone values in the data gaps between SBUV data locations. The BME analysis of total ozone was compared to the TOMS total ozone analysis over the entire domain and with the total ozone analysis derived using a conventional spatial regression interpolation technique (Kriging).

3. RESULTS

Figure 4 shows the analysis of total ozone using the

Table 1 Comparison Statistics (i.e., the Results from the Two Procedures Versus the TOMS Observations) for the 6 July 1988 Case Study.

Procedure	**Bias (DU)**	**Error (DU)**	**R^2**
Kriging	-3.0	7.1	0.45
BME	-0.9	3.7	0.83

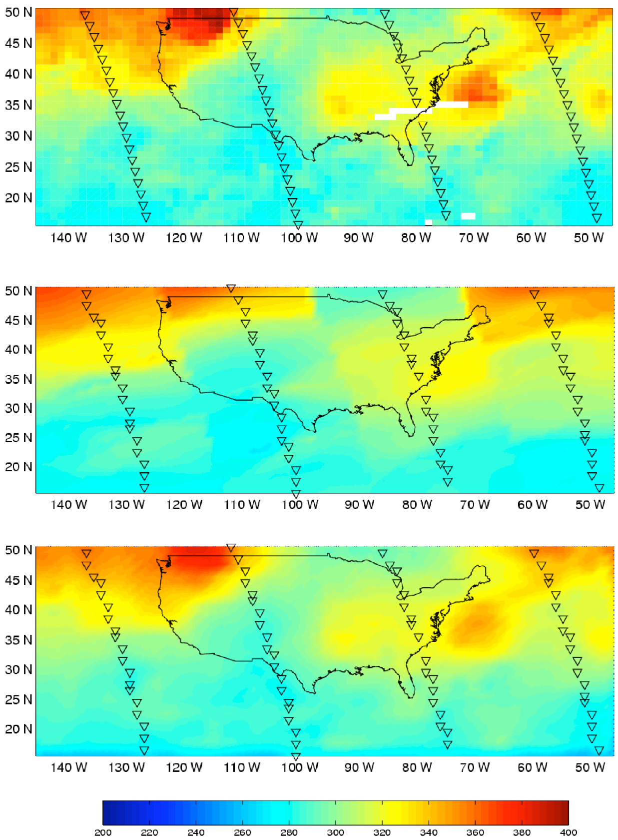

Figure 4 The TOMS total ozone analysis (Top), total ozone analysis applying Kriging (Middle), and total ozone analysis applying BME procedure (Bottom) for 6 July 1988

BME procedure (lower figure), that using Kriging (middle figure), and that using the entire TOMS data set (top figure). Comparison statistics are given in Table 1. There was a 67% improvement in the bias, nearly a 50% improvement in the error, and an 84% improvement in the variance accounted for using the BME procedure. Figure 5 show the error distribution about the SBUV data locations using Kriging (upper figure) and BME (lower figure). For the Kriging analysis, the error increases markedly away from a data location, but for the BME analysis, the error is almost uniform across the analysis.

5. CONCLUSIONS

The usefulness and practicality of using the BME interpolation procedure as a means to interpolate low spatial resolution observations to obtain high spatial resolution analyses of total ozone by integrating data from various information sources (different instruments, empirical laws, uncertain measurements, etc.) into the interpolation procedure has been demonstrated. The BME interpolation procedure integrated sparse data obtained at the locations where SBUV measurements were available with physical knowledge bases, which include the covariance functions (accounting for the variability of ozone values away from the Nimbus 7 satellite path) as well as soft data obtained from the total ozone-tropopause pressure relationship. Application of soft data in the interpolation procedure was critical since it provided a means to incorporate information about the potential variation of ozone in areas where SBUV data gaps were found. Such soft information was rigorously incorporated into the BME interpolation procedure, thus yielding more accurate analyses of total than could be obtained using conventional interpolation techniques.

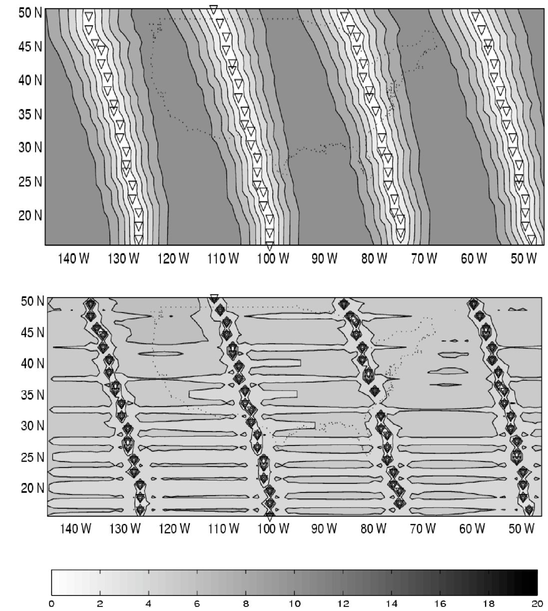

Figure 5 Error distribution for the Kriging (Upper) and BME (lower) analyses.

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