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Non-coincident inter-instrument comparisons of ozone measurements using quasi-conservative coordinates

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Abstract. Ozone measurements from ozonesondes, ARO-TAL, DIAL, and POAM III instruments during the SOLVE-2/VINTERSOL period are composited in a time-varying, flow-following quasi-conservative (PV- θ) coordinate space; the resulting composites from each instrument are mapped onto the other instruments' locations and times. The mapped data are then used to intercompare data from the different instruments. Overall, the four ozone data sets are found to be in good agreement. ARO-TAL shows somewhat lower values below 16 km, and DIAL has a positive bias at the upper limits of its altitude range. These intercomparisons are consistent with those obtained from more conventional near-coincident profiles, where available. Although the PV- θ mapping technique entails larger uncertainties of individual profile differences compared to direct near-coincident comparisons, the ability to include much larger numbers of comparisons can make this technique advantageous.

1 Introduction

The Kiruna deployments of the SOLVE-2 and VINTERSOL field experiments took place in January and February 2003. During this period, a number of different instruments measured stratospheric ozone. On board the NASA DC-8 aircraft were the Airborne Raman Ozone, Temperature, and Aerosol Lidar (AROTAL) and the Differential Absorption Lidar (DIAL), as well as in situ instruments such as FAST response Ozone instrument (FASTOZ) and the Gas and Aerosol Measurement Sensor/Langley Airborne A-Band Spectrometer (GAMS/LAABS). Other instruments, such as the balloon-borne MkIV interferometer, flew on other platforms or took ground-based measurements. A number of sites launched ozonesondes in coordination with the campaigns. In addition, data from the Polar Ozone and Aerosol Measurement III (POAM III) solar occultation instrument on the SPOT-4 spacecraft were made available to the mission teams.

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The usual approach to instrument intercomparisons is to select measurements which were taken at nearly the same time and place. Flying on board the NASA DC-8 together, the AROTAL and DIAL instruments were coincident, and the DC-8 flew over Ny Ålesund in coordination with a number of the sonde launches there. But because many of the instruments operated on different platforms at different times and locations, opportunities for measurement intercomparison were less than plentiful for most instruments. Aside from the AROTAL/DIAL data, the small number of near-coincident measurement sets make a statistical evaluation of inter-instrument differences problematic. Other approaches exist which do not depend on coincidence of the measurements being compared. The trajectory-mapping approach of Morris et al. (2000), the trajectory-hunting method of Danilin et al. (2003), and the MATCH technique of Rex et al. (1999) are examples.

In this work, a quasi-conservative coordinate method is employed. Described in Schoeberl and Lait (1991), this technique depends upon the premise that a reasonably long-lived trace gas should be well-mixed along contours of potential vorticity (PV) on a surface of constant potential temperature (θ) (Leovy et al., 1985). By using PV and θ as coordinates, averaging mixing ratios near a set of points in that coordinate space should yield an accurate picture of a time-invariant trace gas distribution in PV- θ space, in the absence of diabatic effects and chemical changes. In the lower stratosphere at middle to higher latitudes, these latter effects often may safely be ignored for short time periods of approximately 10 days or less. For longer periods, they must be taken into account somehow.

PV- θ analysis was used in Schoeberl et al. (1989), Lait et al. (1990), and Randall et al. (2002) to map measurements onto a three-dimensional field, and in Kyrö et al. (2000) and Lait et al. (2002) to determine stratospheric ozone loss in the Arctic. Lary et al. (1995) used a similar method to initialize model simulations. The quasi-conservative coordinate method can be also useful in inter-instrument comparisons, as seen in Redaelli et al. (1994) and Manney et al. (2001).

In this work, we intercompare ozone measurements from several instruments during the SOLVE-2/VINTERSOL period. Section 2 describes each of these data sets briefly; then the analysis technique is described in Sect. 3. Results follow in Sect. 4.

2 Data

The SOLVE-2/VINTERSOL joint field experiment took place in January through early February 2003. We used data from four instruments: AROTAL, DIAL, POAM III, and the ozonesondes. Measurements were used from January 1 through February 10.

The NASA Goddard Space Flight Center's AROTAL instrument is a lidar that uses Rayleigh scattering from xenon

chloride eximer and Nd:YAG lasers transmitting at 308 and 355 nm to measure ozone, temperature, and aerosols. A more complete discussion of the instrument may be found in McGee et al. (2001) and Burris et al. (2002). For the SOLVE-2/VINTERSOL mission archive, AROTAL reports profiles every 22 s, averaged over 1.2 min. The altitude of the profiles depends on the altitude of the DC-8 aircraft, but over the middle of the flight the data tend to range from approximately 14 km to 35 km. Vertical resolution of the reported data is approximately 150 m. Data were collected for 12 flights of the DC-8. To avoid problems with sunlight increasing noise in the measurements, only profiles taken where the local solar zenith angle is greater than 95° were used.

A second lidar, the NASA Langley Research Center's DIAL instrument, also flew on the DC-8. This instrument uses two Nd:YAG lasers transmitting at multiple frequencies to observe ozone below and above the aircraft. The DIAL data in the mission archive consist of profiles spaced about a minute apart. As with AROTAL, the altitudes covered change with the altitude of the aircraft, but typical coverage is from a few kilometers above the surface to around 25 km, with a small altitude gap near the aircraft itself. Vertical resolution reported is approximately 75 m. Data were collected for 14 flights (including two pre-mission test flights before the deployment to Kiruna). Details of this instrument may be found in Browell et al. (2003), Browell et al. (1998), and Richter et al. (1997).

A total of 214 balloon-launched sonde profiles from 21 ground stations were used in this analysis. These included special sondes launched for VINTERSOL, as well as those launched by the Meteorological Service of Canada, the World Meteorological Organization network, Japan, and Russia. Data were used from the stations shown in Table 1. (Beginning and ending dates shown are confined to the time period examined here.) Altitude ranges vary greatly, but the sondes got as high as 29 km. Reported vertical resolution also varies, from about 10 m to around 60 m.

The POAM III solar occultation instrument is described in Lucke et al. (1999). It is a nine-channel photometer that uses solar occultation to measure atmospheric extinction in bands from 0.354 to 1.018 μm to retrieve temperature and multiple species, including ozone. Fourteen profiles are taken in the Northern Hemisphere each day (as well as fourteen in the Southern Hemisphere), spaced around a latitude circle that moves slowly in time. Vertical resolution is approximately 1 km (Lumpe et al., 2003).

To apply the quasi-conservative coordinate analysis, values of potential vorticity and potential temperature must be obtained at each measurement location and time. For this work, these are obtained by interpolating three-dimensional gridded analyses from the Data Assimilation Office (now the Global Modeling and Assimilation Office) of NASA's Goddard Space Flight Center. These analyses were chosen because of their relatively fine horizontal and temporal resolution, as well as their altitude range. The analyses used

Table 1. Ozonesonde stations

Station	Longitude	Latitude	No.Profiles	Beg. Date	End. Date
Alert	−62.33	82.50	13	Jan. 3	Feb. 10
Churchill	−94.07	58.74	8	Jan. 1	Feb. 5
Eureka	−85.94	79.99	11	Jan. 3	Feb. 10
Goosebay	−60.36	53.31	7	Jan. 8	Feb. 5
Resolute	−94.97	74.71	7	Jan. 2	Feb. 10
Stonyplain	−114.11	53.55	5	Jan. 1	Jan. 29
Hohenpeissenberg	11.00	47.80	17	Jan. 1	Feb. 10
Jokioinen	23.50	60.80	9	Jan. 3	Feb. 8
Sodankyla	26.65	67.39	25	Jan. 1	Feb. 9
Keflavik	−22.60	63.97	9	Jan. 3	Feb. 7
Kuehlungsborn	11.77	54.12	2	Feb. 3	Feb. 4
Legionowo	20.97	52.40	9	Jan. 8	Feb. 5
Lerwick	−1.18	60.13	3	Jan. 5	Jan. 11
Ny Ålesund	11.95	78.93	19	Jan. 6	Feb. 10
Orland	9.24	63.42	6	Jan. 7	Feb. 5
Prague	14.45	50.02	16	Jan. 3	Feb. 10
Scoresbysund	−22.00	70.50	8	Jan. 1	Feb. 7
Thule	−68.74	76.53	5	Jan. 14	Jan. 31
Uccle	4.35	50.8	19	Jan. 3	Feb. 10
Salekhard	66.70	66.70	10	Jan. 4	Feb. 6
Yakutsk	129.63	62.03	6	Jan. 8	Feb. 10

were chosen from the “final look” product generated from the GEOS-4 system. GEOS-4 was the successor to the GEOS-1 system documented by Pfaendtner et al. (1995). These data grids extend from 1000 to 0.2 hPa, have a horizontal resolution of 1.25° longitude by 1.0° latitude, and are produced four times daily.

3 Analysis

In order to derive meaningful statistics for both coincident and non-coincident comparisons, it was necessary to obtain uncertainties associated with the ozone measurements. Such uncertainties are derived from variations of ozone values at a point in PV- θ space. These variations include not only the instruments' random error, but the small-scale geophysical variability that is not resolved by the gridded meteorological analyses. Both sources of variance are needed for this analysis, and an empirical estimation is useful. To estimate the uncertainties for AROTAL and DIAL, a standard variance profile for each instrument was constructed from the small-scale horizontal variations of all the profiles from all flights. For ozonesondes, we used the larger of 5% of the measured value, or the variance about a linear fit within a 5 km segment. However, because small-scale geophysical variability is much less of a problem with the POAM III data, the uncertainties used were taken from the data archive.

The measurements, with their uncertainties, locations, and times were collected for each instrument. (For the sondes, the winds were used to estimate the horizontal location of

each balloon during its ascent.) Modified potential vorticity (see Lait, 1994) and potential temperature were interpolated from the meteorological analysis onto the measurement locations and times.

To aid in the statistical analysis, measurements going into the analysis need to be independent of each other. Data with high horizontal or vertical resolution, however, are highly autocorrelated and must therefore be thinned out. By computing autocorrelations of the lidar data along the flight, we were able to estimate the minimum horizontal separation to ensure independence of profiles as approximately 400 km for AROTAL measurements and 375 km for DIAL. These distances are roughly consistent with those computed by Schoeberl et al. (2002) for the same instruments. Consequently, roughly ten profiles were used from each flight. Because the profile sites for the sondes and POAM III data were widely separated, horizontal separations were not an issue for those instruments. Minimum vertical separations between a profile's measurements were similarly obtained. For AROTAL, the vertical separation was estimated to be 3 km; for DIAL, it was 4 km. For the sondes, it was 3 km, and for POAM data, 4 km.

The analysis itself is similar to that in Lait et al. (2002). A regular grid in a PV- θ coordinate space was constructed, and PV and θ values interpolated from the analyses were used to locate each ozone measurement in the coordinate space. Data from January 1 through February 10 were used; hence, diabatic effects and chemical changes needed to be accounted for. These effects both show up as a change in ozone over

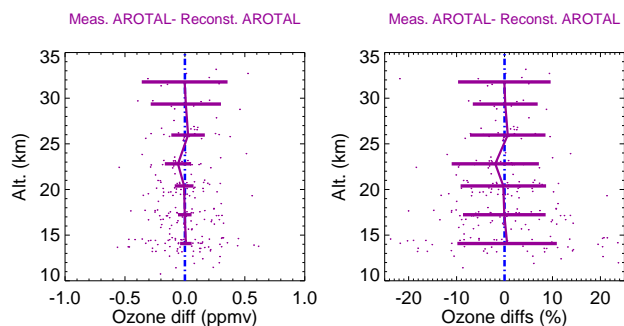


Fig. 1. (left) Self-comparison biases for AROTAL data, expressed as the difference between the original measurements and the measurements reconstructed through PV- θ mapping. Dots are the individual differences, the thin line is the mean difference profile, and the thick horizontal lines are the 90% confidence limits of the mean differences. (right) the differences expressed as percentages of the mean profile.

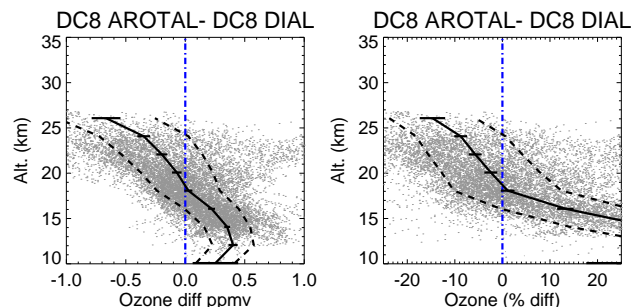


Fig. 2. (Left) Near-coincident differences between AROTAL and DIAL. Gray dots represent individual differences, the solid line shows the mean difference profiles, horizontal lines show the estimated 90% confidence limits of the mean profile, and the dotted lines show the standard deviation of the differences. (Right) The differences expressed as percentages of the mean profile.

time at a given point in PV- θ space. To first order, they can be dealt with by applying a weighted linear time fit to the data near a given PV- θ gridpoint. Each point was weighted inversely to its uncertainty and its distance from the PV- θ gridpoint being examined.

This procedure yields a set of slopes and intercepts, one for each gridpoint in the PV- θ coordinate space. From these, we can construct a composite field in PV- θ space for any moment in time; moreover, given the meteorological analyses we can map this ozone field back into longitude-latitude-altitude space. Note that for instrument comparison purposes here, only the overall evolution of the ozone field is relevant. Whether changes in that field are caused by diabatic effects or by chemical loss/production is of no concern, and so there is no need to try to separate those two effects.

Data from two instruments are compared by constructing a PV- θ composite field from one instrument and mapping

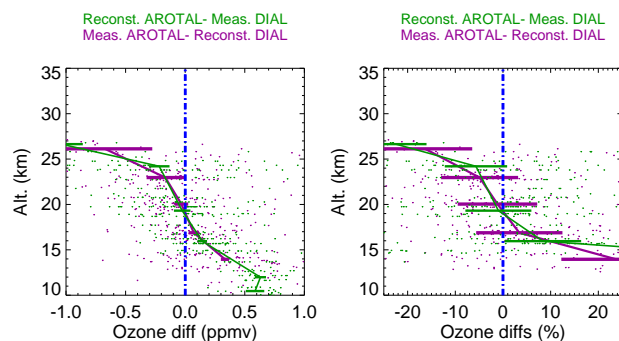


Fig. 3. (Left) Differences between AROTAL and DIAL, using PV- θ analysis. The mean differences (with their 90% confidence limits) are shown for the comparisons both using AROTAL data reconstructed onto DIAL measurement locations (thin green line), and DIAL data mapped onto AROTAL locations (thick purple line). (Right) Differences expressed as percentages of the mean profile.

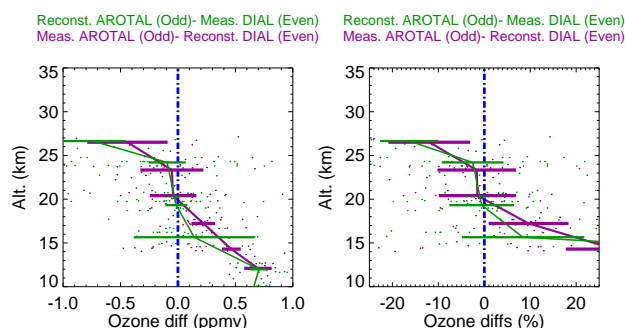


Fig. 4. As in Fig. 3, except that AROTAL data from the odd-numbered DC-8 flights are compared with DIAL data from the even-numbered flights.

its ozone values onto the locations and times of the second instrument. The differences between the two ozone values and the uncertainties associated with those differences are collected, and mean profiles of the biases are computed for the mission period, taking the uncertainties into account.

4 Results

To validate the analysis technique, several tests were applied.

First, each instrument was compared against itself. That is, differences were characterized between the all of the original measurements taken during the time period and those from PV- θ mapping of the same instrument's data. This test should reveal any biases or distortions introduced by the analysis technique itself, and it should also reveal the degree to which noise is introduced by errors in the meteorological fields, departures from assumption of being well-mixed, and so on. Figure 1 shows an example of the self-comparison for AROTAL data. The maximum difference, less than 0.1 ppmv near

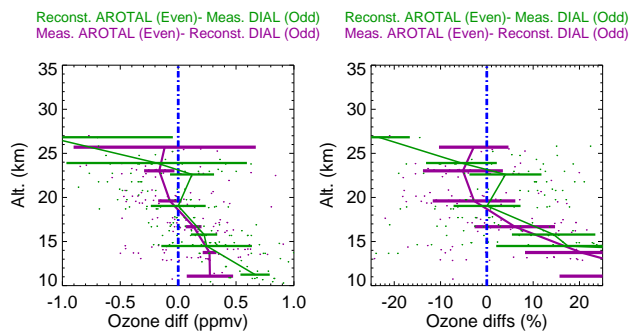


Fig. 5. As in Fig. 3, except that AROTAL data from the even-numbered DC-8 flights are compared with DIAL data from the odd-numbered flights.

22 km, is not statistically different from zero, and the rest of the profile is very close to zero. The self-comparisons for the other instruments show similar results: very small average differences, with at most minor statistically insignificant fluctuations.

The next test was to compute inter-instrument differences between AROTAL and DIAL using both near-coincident and non-coincident methods. Because both these instruments flew aboard the same aircraft, a large number of near-coincident profiles could be collected. For the 12 SOLVE-2 flights of the DC-8, the two closest profiles of the two instruments were chosen within each 400-km flight segment; each profile pair in a flight had to be separated from all other profile pairs by at least 400 km. For each profile pair, the DIAL data were then interpolated to the AROTAL altitudes, and the two profiles were differenced. Figure 2 shows the differences and their average profile. Above 20 km, DIAL ozone values start to become systematically higher than AROTAL – up to 0.7 ppmv higher around 25 km. Below 16 km, AROTAL values are higher, up to 0.4 ppmv higher near 12 km.

Comparing the AROTAL and DIAL data using the non-coincident PV- θ analysis yields similar results (Fig. 3). Note that the measured–reconstructed differences are consistent with the reconstructed–measured differences. Of course, because the data being compared were in fact coincident, this is no more rigorous a test of the noncoincident technique than the self-comparisons. Nevertheless, this comparison is useful for evaluating the success of the next test.

A more demanding test is to compare true non-coincident DIAL and AROTAL data. To accomplish this, AROTAL data from the even-numbered flights were compared with DIAL data from the odd-numbered flights, and vice-versa. The results, shown in Figs. 4 and 5, are consistent with the near-coincident comparisons, albeit with larger uncertainties (since they involved only half the data). Figure 4 matches the full data comparison quite well, while Fig. 5 has greater uncertainties but is still roughly consistent with the others.

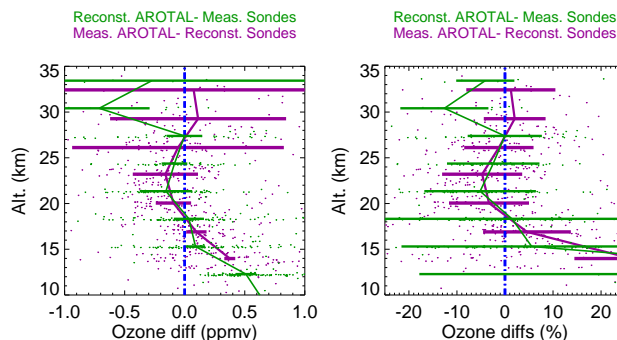


Fig. 6. As in Fig. 3, except that AROTAL data are compared with data from the ozonesondes.

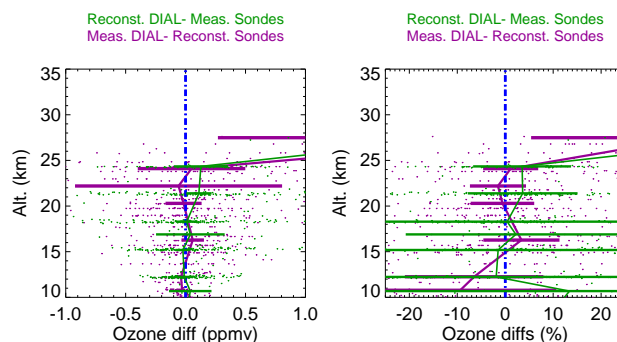


Fig. 7. As in Fig. 3, except that DIAL data are compared with data from the ozonesondes.

Note that the altitude ranges of the two curves in each plot differ. DIAL measures ozone profiles below the aircraft as well as above. However, vertical undulations of isentropic surfaces enable the AROTAL measurements to sample regions of PV- θ space which can be mapped into lower altitudes than the instrument actually measured.

Having confirmed that each instrument's data compare well with themselves, and that the AROTAL–DIAL non-coincident comparisons are similar to the coincident comparisons, we proceeded to compare the other instruments' data.

Figure 6 shows the differences between AROTAL and the ozonesondes. There appears to be a bias below 15 km, with AROTAL being perhaps 0.3 to 0.4 ppmv higher than the sondes near 12–13 km. Above 25 km, the ozonesondes are fewer in number and their uncertainties are often larger, so that the error bars in the differences are much larger at those altitudes. Nevertheless, there is some suggestion of AROTAL data being systematically lower than the sondes at these altitudes. (Note also the error bars in the percentage plot depend on the variance in the mean profile as well as the mean difference, and the resulting uncertainties are larger at lower altitudes as a result.)

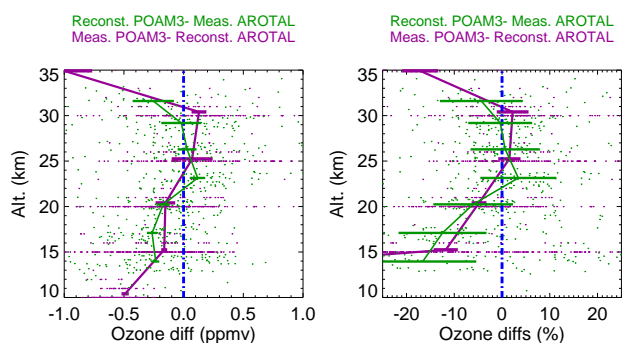


Fig. 8. As in Fig. 3, except that AROTAL data are compared with data from POAM III.

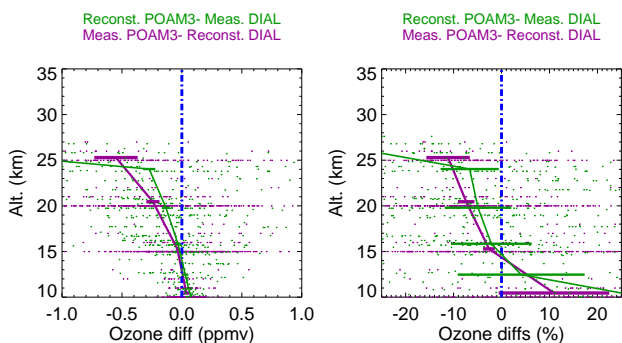


Fig. 9. As in Fig. 3, except that DIAL data are compared with data from POAM III.

Likewise, the differences between DIAL and the sondes is shown in Fig. 7. Here, DIAL matches the sondes well at the lower altitudes, but DIAL is higher at the uppermost reaches of the instrument, above 25 km. This is only one altitude, however, and it is associated with a large uncertainty. But the AROTAL-sonde and DIAL-sonde differences are consistent with the AROTAL-DIAL differences.

Figures 8 and 9 show the POAM-AROTAL and POAM-DIAL differences, respectively. The POAM-AROTAL differences are qualitatively similar to biases noted in Lumpe et al. (2003), where coincident comparisons were made between POAM III and AROTEL (an earlier version of AROTAL) and DIAL during the first SOLVE campaign in the winter of 1999–2000. The POAM-DIAL differences at the uppermost DIAL altitudes, however, are of different sign from those in Lumpe et al. (2003).

Figure 10 compares the ozonesonde data with the POAM III profiles. The two data sets agree below 18 km, but a possible small bias appears near 20 km, with the sondes being about 0.2 ppmv higher. At higher altitudes, between 25 and 30 km, there is also a suggestion of a small positive bias of 0.2 ppmv, relative to the sondes, but the sonde measurements are fewer and less certain here. Using coincident comparisons, Randall et al. (2002) found no systematic bias

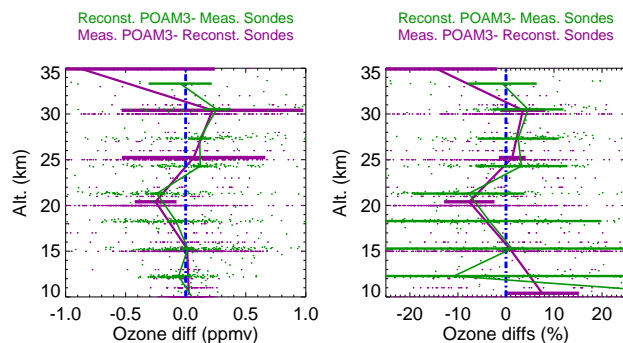


Fig. 10. As in Fig. 3, except that ozonesonde data are compared with data from POAM III.

between sondes and POAM between 13 to 60 km, but they did find evidence for a 0.1 ppmv positive POAM bias between 10 to 12 km,

These intercomparisons were repeated with other meteorological analyses (UARS UKMO Assimilation, NCAR/NCEP Reanalysis, and NCEP Spectral Statistical Interpolation products); the results were similar.

5 Conclusions

Ozone measurements taken during the SOLVE-2/VINTERSOL field experiment from four instruments (AROTAL, DIAL, POAM III, and sondes) were compared. A quasi-conservative coordinate approach was employed to use non-coincident data for instrument intercomparisons. Several tests of the method were applied. First, each instrument's data were self-compared; the differences were zero, within the uncertainty associated with the technique. Second, the AROTAL and DIAL data were compared, with results similar to those from the straightforward near-coincident comparison. These tests demonstrate that the quasi-conservative technique does not introduce unusual or misleading artifacts into the data. To provide a true non-coincident data comparison, the DIAL data from the odd-numbered DC-8 flights were compared with AROTAL data from the even-numbered flights, and vice versa. These results were consistent with the other DIAL-AROTAL comparisons, although the uncertainties were larger.

Finally, all four data sets were intercompared. By finding commonalities among the intercomparisons, it is possible to determine which instruments exhibit systematic biases at which altitudes. The AROTAL data exhibit a positive bias of 0.3 to 0.7 ppmv at altitudes below 16 km (roughly 20% at those altitudes), when compared to DIAL, the sondes, and POAM. DIAL, however, shows a positive bias of 0.5 to 1.0 ppmv (15–20%) at its uppermost altitude range (above 25 km), when compared to AROTAL, POAM, and perhaps the sondes. AROTAL and DIAL agree within 0.25 ppmv, or better than 10%, from about 17 km to 22 km, according to

the coincident comparisons; this is consistent with the non-coincident comparisons.

The ozonesonde and POAM data appear to be of very good quality, on average. The two match each other well, except for a possible small bias in a region near 20 km. DIAL compares very well with the sonde data (better than 5%) between 13 and 25 km, consistent with the DIAL/POAM comparison. AROTAL, too, compares well (6% or better) with POAM and the sondes above around 20 km, up to 30 km, although the POAM/AROTAL comparisons suggest a high bias for AROTAL at its highest altitudes.

This PV- θ analysis produces results with substantial uncertainties. The uncertainties associated with the limited-resolution analyzed PV and θ meteorological fields, limited sampling over regions of PV- θ space, potential failures in the assumptions necessary for the method's validity (e.g. homogeneity around a circumpolar PV- θ tube), and even a breakdown in PV-ozone correlations at high altitudes and low latitudes, can all contribute to the enlarged error bars. Certainly, then, direct comparison of large numbers of near-coincident measurements is preferred where it is possible. Nevertheless, the higher numbers of comparisons which are made possible by relaxing the requirement for near-coincidence, can improve the statistics so that the results are useful despite their uncertainties.

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