On the Application of the Optimum Statistical Inversion Technique to the Evaluation of Umkehr Observations

JOHN J. DELUISI AND CARLTON L. MATEER[1]

National Center for Atmospheric Research[2], Boulder, Colo.

(Manuscript received 1 September 1970, in revised form 2 November 1970)

ABSTRACT

The optimum statistical inversion technique is applied to the evaluation of Umkehr observations from Arosa (46.5N, 9.4E), Aspendale (38.0S, 145.1E) and Tallahassee (30.2N, 84.2W). *A priori* statistical information on the vertical ozone distribution is obtained from 511 balloon-sounding profiles at Boulder (40.0N, 105.1W). These latter data are also used to develop a regression method for obtaining a first guess at the O_3 distribution, using total O_3 as the independent variable. The ozone profiles inferred from the statistical method, when compared with concurrent direct measurements, display a significant improvement over profiles derived by the method in use at the World Ozone Data Center. Most of this improvement is attributable to the better first guess based on the total O_3 regression. It is concluded that the utility of Umkehr observations is mainly restricted to estimation of the high-level O_3 distribution above the main O_3 maximum. For inferences about the ozone distribution at and below the maximum, effort should be directed toward regression techniques using total ozone as the independent variable.

1. Introduction

The standard method now in use by the World Ozone Data Center at Toronto for estimating the vertical ozone distribution from Umkehr observations[3] was developed by Mateer and Dütsch (1964). Comparisons between ozone distributions obtained in this manner and those measured by balloonborne ozonesondes at nearly the same time and location have been reported by Mateer and Dütsch (1964), Bojkov (1966), Craig *et al.* (1967), and Dütsch and Ling (1969). These comparisons have all shown that the Umkehr-derived distributions display, on the average, too little ozone at and near the main maximum, and too much ozone at lower levels in the atmosphere. DeLuisi (1969) has shown that part of the discrepancy could be attributed to the neglect of scattering by haze in the evaluation model. Dütsch and Ling (1969) have suggested that part of the difference could be due to an excessive smoothing effect of the indirect method.

The application of *a priori* statistical information on the vertical O_3 distribution to the Umkehr evaluation was first attempted by Mateer (1964), who expanded the vertical distribution in terms of empirical orthogonal functions. Although the results appeared promising, the method was not followed in development of the standard procedure because of the lack of a sufficiently large statistical sample of O_3 sounding results. In the present paper, we report on results achieved by the application of the optimum statistical inversion procedure which was developed independently by Rodgers (1966) and Strand and Westwater (1968).

2. The evaluation model

The evaluation model is very similar to that of Dütsch (1957, 1959) and Mateer and Dütsch (1964). We use the truncated Taylor expansion of the Umkehr N value, which may be written as

$$N_k = U_k + \sum_{i=1}^{m} \frac{\partial U_k}{\partial f_i} \Delta f_i, \quad (1)$$

where N_k is the observed N value for the kth zenith angle, U_k the N value for the kth zenith angle as computed for a standard or first-guess ozone distribution, f_i the logarithm of the amount of ozone in the ith layer of the standard distribution, Δf_i the logarithm of the ratio of the ozone amount in the ith layer of the solution

[1] Present affiliation: Canadian Meteorological Service, Toronto, Canada.

[2] The National Center for Atmospheric Research is sponsored by the National Science Foundation.

[3] Umkehr observations consist of a series of measurements of the ratio of the zenith sky light intensities of two wavelengths in the solar ultraviolet while the sun is between 0° and 30° above the horizon. The double monochromator used for these measurements is calibrated to give the logarithm (base 10) of the ratio of the intensity of the shorter (strongly absorbed) wavelength to the intensity of the longer (weakly absorbed) wavelength. The calibration includes an allowance for the ratio of the extraterrestrial solar fluxes at the two wavelengths. Accordingly, the data give the relative logarithmic attenuation for the diffuse transmission of the two wavelengths through the atmosphere. The so-called N value gives this relative logarithmic attenuation in units of 10^{-2} bel = 1 centibel (cb).

to the ozone amount in the ith layer of the standard distribution, and m the number of layers in the evaluation model.

For solution purposes, the atmosphere is divided into 16 layers, the first extending from the earth's surface to 250 mb. The second through sixteenth layers have the property that the ratio of the pressure at the bottom of a layer to that at the top is $2^{\frac{1}{2}}$. The ozone amount above the top of the 16th layer is a fixed fraction of the amount in the 16th layer. Twelve points, representing measurements at zenith angles between 60° and 90°, are selected to represent the Umkehr curve. In order to eliminate a small instrumental constant, we follow the customary procedure of subtracting the observed N value at the smallest zenith angle from each of the other observations.

Using the notation of Strand and Westwater (1968), the solution of (1) under the optimum statistical inversion procedure takes the form

$$\Delta\mathbf{f}=\mathbf{S}_x\mathbf{A}^*(\mathbf{S}_\epsilon+\mathbf{A}\mathbf{S}_x\mathbf{A}^*)^{-1}\mathbf{h}, \qquad (2)$$

where $\Delta\mathbf{f}$ is the maximum likelihood estimate vector of the Δf_i in (1), $\mathbf{A}$ the matrix of partial derivatives (the asterisk superscript denotes matrix transposition), $\mathbf{h}$ the vector of measurements from the Umkehr curve, N_k-U_k in (1), $\mathbf{S}_x$ the covariance matrix of prior information on the Δf_i, and $\mathbf{S}_\epsilon$ the covariance matrix of the errors in Umkehr observations.

3. Derivation of quantities used

To treat total O_3 in an essentially continuous manner, we computed standard N values and their first-order partial derivatives for five O_3 distributions (Fig. 1) which were estimated statistically by a log-linear regression method (see Appendix) using total ozone as the independent variable. This procedure allows us to interpolate the smoothly varying standard N values and their derivatives for any specified total O_3 amount.

The statistical sample of vertical O_3 distributions comprises 511 profiles measured at Boulder, Colo., using the Brewer-Mast ozonesonde (Dütsch, 1966). The typical ozone sounding reaches a height of ~30 km. Since the region above this level cannot be disregarded, the mean distribution for Boulder was smoothly extended upward so that above 45 km it became essentially that used by Dütsch (1959). Then, individual O_3 distributions are smoothly interpolated onto this distribution beginning at the maximum level reached by the balloon and extending up to 45 km.

a. N value and partial derivative calculations

A new method was used for calculating the intensity and partial derivatives of solar ultraviolet radiation diffusely transmitted in the zenith direction in a nonhomogeneous, Rayleigh atmosphere with sphericity. This method is a modification of the auxiliary equation iteration method developed by Dave (1964) for a nonhomogeneous plane-parallel atmosphere. In keeping with the statement by Sekera and Dave (1961) that most of the multiply scattered light comes from a rather narrow cone about the zenith direction, we considered the sphericity effects to be important only for the primary-scattered light. Therefore, Dave's zero-iteration values, which represent the primary-scattered photons, were computed for a spherical atmosphere, and the second and higher orders were computed for the plane-parallel atmosphere by successive iteration of these zero-iteration values. This may be referred to as the pseudo-spherical atmosphere.

To obtain an estimate of the accuracy of this method, we compared secondary scattering intensities computed for a spherical atmosphere with those computed by the above procedure. In general, the differences were less than 1–2%, except for the sun on the horizon for the longer Umkehr wavelength (3323 Å) which is only weakly absorbed by O_3. In this latter case, the difference

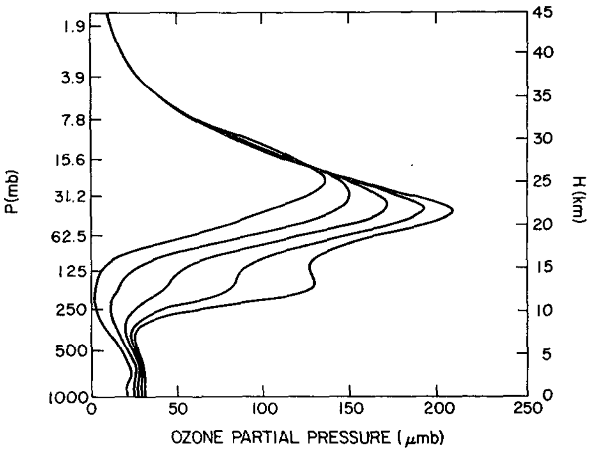

FIG. 1. Standard vertical ozone distributions for total integrated ozone amounts of 0.240, 0.290, 0.340, 0.390 and 0.440 cm (STP). The gradations on the pressure axis are for the layer system used by the World Ozone Data Center.

TABLE 1. Variance [(log$_e$)^2] of Boulder ozone distributions after application of the total ozone regression.

Layer	Variance
1	0.0814
2	0.3763
3	0.2529
4	0.1332
5	0.0430
6	0.0194
7	0.0109
8	0.0059
9	0.0107
10	0.0205
11	0.0263
12	0.0260
13	0.0185
14	0.0100
15	0.0041
16	0.0008

TABLE 2. Average and variance of empirical adjustment to observed Umkehr curves at various locations.

Solar zenith angles (deg)	Arosa Average (cb)	Arosa Variance (cb)²	Aspendale Average (cb)	Aspendale Variance (cb)²	Tallahassee Average (cb)	Tallahassee Variance (cb)²	Haze effect (cb)
65	−0.10	0.27	*	*	0.10	0.18	−0.15
70	−0.22	1.00	*	*	0.07	0.58	−0.45
74	−0.45	1.95	−0.23	0.44	−0.07	1.12	−0.90
77	−0.78	3.47	−0.34	0.76	−0.27	1.77	−1.44
80	−0.91	4.94	−0.31	1.68	0.10	2.44	−1.95
83	−0.22	8.12	1.14	4.00	1.00	4.73	−1.73
85	0.96	7.83	2.97	6.48	2.63	5.87	−1.34
86.5	1.69	8.01	4.41	8.47	3.96	6.02	−0.72
88	2.27	8.80	5.48	12.04	4.63	5.22	−0.40
89	1.93	10.17	5.61	13.58	4.18	4.11	−0.42
90	0.81	11.06	5.06	16.15	3.23	3.22	−0.56

* The smallest zenith angle available for all Umkehrs at Aspendale is 70°. The N value at 70° is subtracted from the N values at the remaining zenith angles to remove the instrumental constant.

was nearly 3%. Since each higher order of scattering contributes a proportionately lesser amount to the total intensity (at least in the present problem), we consider that the error due to this cause in our standard N values should not exceed about 0.7 cb at zero sun-height, which is the "worst case."

The partial derivatives were obtained by computations based on the differentiation of the numerical expressions used for the intensity calculation.

b. *A priori statistical information*

In the present procedure, the matrix $\mathbf{S}_x$ represents the covariance of the O_3 distribution remaining after application of the log-linear regression based on total ozone. Accordingly, we obtained an estimate of $\mathbf{S}_x$ from the differences between the 511 Boulder soundings and the corresponding regression distributions. The diagonal elements of $\mathbf{S}_x$ are listed in Table 1. As one would expect, the greatest variability is in the lower stratosphere. However, there is a small secondary peak in variability in layers 11 and 12 which are at the ceiling of the balloon soundings. It is not certain whether this peak is real or whether it is due to an increase in the random errors of the direct sounding method, possibly due to differences in the degree of lubrication of the air pumps in the different ozonesonde units (see Komhyr and Harris, 1965). Certainly, from the photochemical theory, one would expect the variability between soundings to gradually decrease with increasing height as the time for equilibrium to be reached also decreases. Finally, since the individual profiles in our sample have been forced to merge to a common profile above layer 16, the gradual decrease in variance above layer 12 is also forced.

c. *Concurrent data samples*

The concurrent data comprise three sets: 49 cases for Arosa (46.5N, 9.4E), 33 for Aspendale (38.0S, 145.1E), and 39 for Tallahassee (30.2N, 84.2W). By concurrent, we mean that an ozonesonde and an Umkehr observation (C-wavelength pair) have been made during the same day, or an evening observation of one type is paired with one of the other types made the following morning. A few of the Tallahassee observations have a morning and an evening Umkehr for a single ozonesonde flight taken on the same day. At Tallahassee and Aspendale, both the Umkehr and the concurrent sonde data are for the same location. However, the Arosa Umkehrs are paired with direct measurements at Thalwil ~60 mi northwest of Arosa.

The direct measurements of ozone distribution at Arosa and Aspendale were made with the Brewer-Mast ozonesonde (Brewer and Milford, 1960), while those at Tallahassee were made with the chemiluminescent ozonesonde (Regener, 1964). Both types of instrument suffer from errors and the measured profiles have to be adjusted to agree with the directly measured total integrated O_3. In addition, O_3 profiles obtained with the Brewer-Mast instrument require a correction for loss in pump efficiency above ~150 mb (Komhyr and Harris, 1965). Komhyr *et al.* (1968) and Powell and Simmons (1969) discuss some of the causes of error for the two types of instrument.

d. *The error matrix*

The evaluation system as embodied in our mathematical-physical model represented by (1) does not account for factors such as scattering and absorption by haze, the temperature dependence of the O_3 absorption coefficients, atmospheric refraction, ground reflection, nonlinearities introduced by the use of (1), and instrumental errors of measurement. In addition, since we use

TABLE 3. Vertical ozone distribution at Arosa in terms of layer-mean ozone partial pressures for a sample size of 49.

Layer	Measured average (μmb)	Total ozone regression Average (μmb)	Total ozone regression rms (μmb)	Solution 1)* Average (μmb)	Solution 1)* rms (μmb)	Solution 2)* Average (μmb)	Solution 2)* rms (μmb)
1	25.5	23.8	7.0	29.9	8.2	25.9	6.6
2	41.8	32.1	20.3	41.2	18.4	36.7	17.6
3	59.9	44.1	23.9	43.8	24.4	45.5	23.8
4	74.1	60.1	21.2	57.1	22.0	61.5	18.9
5	108.4	101.3	17.9	89.2	22.8	100.4	14.8
6	139.8	146.3	16.6	130.1	16.3	143.0	13.3
7	151.6	163.7	16.8	150.0	11.4	160.4	14.3
8	137.7	150.1	15.5	141.4	10.2	146.4	12.9
9	114.8	124.1	12.9	121.9	10.1	119.7	8.8
10	89.2	94.8	11.0	98.5	11.6	91.3	7.3
11	65.8	68.7	7.9	74.6	10.3	66.8	5.4
12	46.8	47.6	6.0	52.0	7.0	46.7	4.6
13	32.1	31.8	4.2	34.2	4.2	31.4	3.7
14	21.1	21.0	2.0	22.1	2.0	20.8	1.8
15	13.6	13.6	0.8	14.1	0.8	13.5	0.7
16	8.7	8.6	0.2	8.8	0.2	8.6	0.2
Total ozone (atm-cm)	0.329	0.329	—	0.327	—	0.327	—
Overall rms error, layers 1–11 ($\log_e$)	—	—	0.298	—	0.280	—	0.255

* See text p. 331.

the Boulder $\mathbf{S}_x$ matrix to evaluate Umkehr data for other locations and since the standard N values and their partial derivatives have been computed for Boulder, certain geographical effects such as station elevation and variations in the statistical properties of the vertical O_3 distribution are not accounted for in the evaluation procedure. In effect, all of these factors enter into the error matrix $\mathbf{S}_\epsilon$.

Although the effect of each of these factors may be estimated separately, an alternative and much simpler method is to calculate $\mathbf{S}_\epsilon$ empirically by using the directly measured ozone distributions to construct Umkehr curves from (1). These curves may then be subtracted from the concurrently measured Umkehr curves and the differences used to compute, for each concurrent sample, the error covariance matrix $\mathbf{S}_\epsilon$ and an average adjustment to the observed Umkehr curve to make it compatible with the basic tables used in the inversion procedure.

These average adjustments and the corresponding diagonal elements of $\mathbf{S}_\epsilon$ are listed in Table 2 for each concurrent sample. Since the average adjustments are calculated by a method very similar to that used for DeLuisi's (1969) "haze effect" curve, the latter is shown in the extreme right column of Table 2. The differences between DeLuisi's haze effect and the present results appear rather large. We have determined that the differences are primarily caused by the method we used to smoothly join the top point of the average Boulder balloon sounding to Dütsch's ozone distribution above 45 km. Furthermore, this average sounding was used at other geographical locations. In the earlier work by DeLuisi, there was more O_3 between 30 and 45 km in

TABLE 4. Vertical ozone distribution at Aspendale in terms of layer-mean ozone partial pressures for a sample size of 33.

Layer	Measured average (μmb)	Total ozone regression Average (μmb)	Total ozone regression rms (μmb)	Solution 1) Average (μmb)	Solution 1) rms (μmb)	Solution 2) Average (μmb)	Solution 2) rms (μmb)
1	22.9	22.2	3.9	28.4	7.1	23.2	3.8
2	31.4	23.2	15.7	31.5	9.3	25.2	11.4
3	37.0	32.8	16.0	34.5	13.7	33.5	13.7
4	48.2	49.7	13.7	49.4	12.1	50.5	12.2
5	92.5	92.3	14.0	82.6	18.8	93.5	15.7
6	138.2	137.5	13.3	122.4	19.9	138.1	11.9
7	157.0	157.4	11.8	143.5	16.7	157.5	9.6
8	149.5	148.3	12.2	138.4	15.8	147.1	11.6
9	126.1	124.2	14.3	120.2	13.1	121.1	12.7
10	92.4	95.4	12.0	97.2	9.2	91.8	7.9
11	63.3	69.0	10.4	73.5	12.3	66.1	7.5
12	43.3	47.7	7.5	51.2	9.6	45.8	6.0
13	29.4	31.9	4.1	33.8	5.4	30.8	3.3
14	19.8	21.0	2.0	21.9	2.6	20.5	1.6
15	13.1	13.6	0.8	14.0	1.1	13.4	0.6
16	8.5	8.6	0.2	8.7	0.3	8.6	0.2
Total ozone (atm-cm)	0.316	0.316	—	0.315	—	0.315	—
Overall rms error, layers 1–11 ($\log_e$)	—	—	0.256	—	0.220	—	0.205

TABLE 5. Vertical ozone distribution at Tallahassee in terms of layer-mean ozone partial pressures for a sample size of 39.

Layer	Measured average (μmb)	Total ozone regression Average (μmb)	Total ozone regression rms (μmb)	Solution 1) Average (μmb)	Solution 1) rms (μmb)	Solution 2) Average (μmb)	Solution 2) rms (μmb)
1	19.8	21.4	8.2	26.0	9.0	21.1	6.7
2	19.7	19.0	10.4	22.7	10.7	17.4	10.2
3	24.7	27.4	11.8	28.4	9.7	25.4	9.7
4	40.4	44.4	14.0	44.0	11.5	42.9	11.7
5	80.5	87.3	15.5	77.3	12.7	87.7	13.7
6	135.5	132.6	15.6	117.0	22.8	134.3	12.3
7	164.8	153.7	20.7	139.0	29.9	155.6	18.4
8	157.0	147.2	14.2	138.2	20.9	148.6	13.0
9	125.7	124.3	12.0	124.8	9.0	124.9	9.2
10	92.7	95.7	14.6	103.9	15.8	95.5	11.9
11	67.3	69.2	9.5	79.3	14.0	68.6	7.5
12	46.9	47.8	5.4	55.2	9.4	47.4	4.5
13	31.4	31.9	2.8	35.9	5.1	31.7	2.4
14	20.8	21.0	1.3	22.9	2.4	20.9	1.1
15	13.6	13.6	0.5	14.4	1.0	13.6	0.5
16	8.6	8.6	0.1	8.9	0.2	8.6	0.1
Total ozone (atm-cm)	0.308	0.308	—	0.310	—	0.307	—
Overall rms error, layers 1–11 ($\log_e$)	—	—	0.305	—	0.306	—	0.269

the extended Tallahassee soundings because in this region he interpolated the average Tallahassee sounding onto a distribution that was essentially the one used by Dütsch (1957).

Because of the uncertainties in the balloon soundings above the main O_3 maximum, where the pump correction becomes fairly large and less reliable, we believe that the Umkehr results constitute a better estimate of the actual O_3 distribution near the top of the balloon sounding. Consequently, we believe that the $\mathbf{S}_\epsilon$ derived above, representing the variance of Umkehr curve differences about the mean difference, provides a realistic estimate of the random uncertainties between the Umkehr and the direct measurements. Accordingly, we have carried out solutions by two methods, *viz.*, 1) using the above $\mathbf{S}_\epsilon$ on the actual Umkehr data, and 2) using the above $\mathbf{S}_\epsilon$ on Umkehr data adjusted by subtraction of the mean adjustors shown in Table 2. Solutions by 2) will provide a measure of how well the solution procedure can reproduce the assumed distributions, while those by 1) should provide a better indication of the actual high-level distribution because they are not biased by the uncertainties in the balloon soundings above the main ozone maximum.

4. Presentation and discussion of results

Results for Arosa, Aspendale and Tallahassee are presented in Tables 3, 4 and 5, respectively. In each table, the second column shows the average vertical O_3 distribution in terms of the average O_3 partial pressures (μmb) in each layer. The third, fifth and seventh columns give average solutions for the total O_3 regression, solution 1), and solution 2), respectively. The

TABLE 6. Comparison of average ozone distributions given by the World Ozone Data Center (WODC) and the present method. Values are in terms of 100 (Umkehr −direct)/direct.

Layer number	Arosa (49 cases) WODC	Arosa (49 cases) Present	Aspendale (33 cases) WODC*	Aspendale (33 cases) Present	Tallahassee (39 cases) WODC**	Tallahassee (39 cases) Present
1	+35	+17	+47	+24	+42	+32
2	+20	−17	+43	−4	+33	+15
3	−17	−20	+14	−6	−7	0
4	−21	−4	−10	−10	−23	−15
5	−5	+4	+7	−6	−1	−7
6	+19	+12	—	+10	+29	+11

* Results obtained from Pittock and Kulkarni by private communication.
** Results according to Craig *et al.* (1967) for 49 cases.

fourth, sixth and eighth columns give the rms errors for these respective solution methods. At the bottom of each "average" column is shown the corresponding average total O_3 while at the bottom of each rms column is shown the overall rms error, applicable to layers 1–11, in terms of Δf, i.e., natural log units. This latter quantity provides a measure of the average fractional error in the layers for which the balloon sounding data are available.

An examination of the tables reveals that it is not possible to improve a great deal on the first guess obtained from the total ozone regression, at least in layers 1–11. This is particularly true at Aspendale where the first guess is exceptionally good on the average for layers 1–9.

For all locations, application of the respective average adjustment brings the average solution 1) closer to the measured, but assumed to be true, ozone distribution. The change is most pronounced above the maximum. The adjustment also reduces the rms error slightly.

The average solution 1) for all locations adds still more O_3 above the maximum (starting with layer 10) than what is estimated from the first guess. On the other hand, the average solution 2) closely reproduces the average "measured" distribution, as one would expect

TABLE 7. Comparison of correlations of ozonesonde and Umkehr observations for World Ozone Data Center (WODC) and the present Umkehr inversion systems.

Layer number	Arosa (49 cases) WODC	Arosa (49 cases) Present	Aspendale (33 cases) WODC*	Aspendale (33 cases) Present	Tallahassee (39 cases) WODC**	Tallahassee (39 cases) Present
	Correlation coefficients					
1	0.38	0.49	0.47	0.63	0.03, −0.02	0.65
2	0.86	0.89	0.84	0.88	0.56	0.78
3	0.85	0.89	0.82	0.86	0.75	0.90
4	0.79	0.85	0.88	0.87	0.42	0.56
5	0.20	0.59	0.37	0.54	0.28	0.63
6	0.14	0.69	—	0.69	0.54	0.51

* From Pittock (1970).
** From Craig *et al.* (1967) for 49 cases. Layer 1 correlations are for 1000–500 and 500–250 mb layers.

from the design of this technique. The only plausible explanation seems to be that there must be more O_3 above the maximum than what is given by our assumed "true" distribution. This being the case then, there is also in general too much O_3 at and below the maximum in the ozone sounding results because of the procedure of adjusting these soundings to give the correct total ozone. Solution 1) shows this for Tallahassee and Aspendale, but for Arosa there is more O_3 than what is given by the true distribution starting with layer 8; however, this may partially be due to a poor first guess.

Average total O_3 for both solutions is reasonably well conserved at all locations differing at most by ± 0.002 atm-cm. Individual solutions rarely exceeded a difference of ± 0.005 atm-cm. Adequate *a priori* information would most likely reduce these differences.

Another conclusion from the results of the present investigation is that we see no evidence to support the suggestion by Dütsch and Ling that errors in the World Ozone Data Center (WODC) method were caused by excessive smoothing inherent in the indirect method. The lack of a sufficiently pronounced maximum in the WODC results is for the most part due to a deficiency in the standard O_3 distributions used as the first guess. Note in our results that solution 2) reveals a deficit of O_3 at the maximum for Tallahassee and a surplus for Arosa, while Aspendale is nearly coincident, and these remaining deficiencies could be corrected by a better first-guess procedure at each location.

It is necessary to establish whether or not the solutions 1) and 2) represent an improvement over the solutions obtained at the WODC. The method of comparison follows the general procedures used by previous authors who made comparisons between WODC results and balloon sounding distributions, *viz.*, (i) by comparing average O_3 in each layer, and (ii) by computing correlations of the layer concentrations between the two sets of data.

The WODC system uses only nine layers, wherein their first layer is identical to ours, their second layer includes our second and third layers, etc. Consequently, we may compare results by averaging the two partial pressures in our system to convert to the single layer of the WODC system. Table 6 shows the average difference between Umkehr solution 1) and WODC results and the direct measurements, expressed as a percentage of the direct measurement. It is clear that solution 1) provides a significant improvement over WODC.

Table 7 shows results of the correlation comparison. From these results, we note that solution 1) correlations are slightly higher than WODC correlations at all locations except for layer 4 for Aspendale and layer 6 for Tallahassee.

5. Summary and conclusions

Vertical ozone distributions inferred from Umkehr observations by means of the optimum statistical inversion procedure provide a significant improvement over those derived by the standard method in use at the World Ozone Data Center. However, most of this improvement may be attributed to the use of better standard (or first-guess) ozone distributions since the optimum procedure gives only a small improvement over O_3 profiles derived from the total O_3 regression. Because the direct sounding results become increasingly less reliable above the main ozone maximum, Umkehr results are believed to give a more accurate estimate of O_3 partial pressures near 30 km. In particular, these results suggest that the direct soundings at Arosa, Aspendale and Tallahassee indicate too little O_3 in this region.

We conclude that the main usefulness of Umkehr observations in the immediate future will be in the inference of the high-level ozone distribution above the main maximum (see Mateer, 1965). For inferences about the O_3 distribution at and below the main maximum, in the absence of direct balloon soundings, efforts should be directed toward the development and improvement of regression techniques which employ total O_3 as the independent variable. A similar conclusion has been reached by Sellers and Yarger (1969) in a study of the potential utility of satellite measurements of backscattered solar ultraviolet radiation.

Acknowledgments. We are indebted to Prof. H. U. Dütsch at Arosa, to Drs. A. B. Pittock and R. N. Kulkarni at Aspendale, and to Prof. R. A. Craig at Tallahassee for supplying the data. We also wish to thank Dr. W. L. Godson for critical comment on an earlier version of the manuscript.

APPENDIX

Log-Linear Regression on Total Ozone

Ozone distributions for the 16-layer model are derived from the relationship

$$\chi_i = \exp[A_i + B_i(\Omega - 0.343)], \tag{A1}$$

TABLE 8. Regression coefficients for the 16-layer model.

Layer	A_i	B_i
1	−3.6452	3.4619
2	−4.8878	14.925
3	−4.5418	13.710
4	−4.1478	9.2215
5	−3.5824	4.7932
6	−3.2101	3.2363
7	−3.0971	2.1213
8	−3.1879	0.68377
9	−3.3824	−0.051858
10	−3.6537	−0.32339
11	−3.9756	−0.26772
12	−4.3417	−0.17259
13	−4.7455	−0.14598
14	−5.1612	−0.10788
15	−5.5941	−0.069314
16	−6.0475	−0.030729

where χ_i is the ozone amount (atm-cm) in the ith layer, Ω the total ozone (atm-cm), and A_i, B_i the regression coefficients (listed in Table 8).

The total ozone for a distribution derived from (A1) is generally a little different from the input value Ω. To overcome this inconsistency, the Ω used in (A1) is changed iteratively according to

$$\Omega_{j+1} = \Omega_j + 0.5(\Omega_0 - \hat{\Omega}_j), \tag{A2}$$

where Ω_j is the total ozone value used in (A1) on the jth iteration, Ω_0 the actual total ozone, and $\hat{\Omega}_j$ the integrated ozone from (A1) on the jth iteration.

Two or three iterations are usually sufficient to reduce $|\Omega_0 - \hat{\Omega}_j| \leqslant 0.0005$ atm-cm which is quite adequate for our purposes. When summing the χ_i to get total ozone, 0.0038 atm-cm is added for the ozone above the top of layer 16.

REFERENCES

Bojkov, R. D., 1966: Differences in the vertical ozone distribution deduced from Umkehr and ozonesonde data at Goose Bay. *J. Appl. Meteor.*, **5**, 872–877.

Brewer, A. W., and J. R. Milford, 1960: The Oxford Kew ozonesonde. *Proc. Roy. Soc. London*, **A256**, 470–495.

Craig, R. A., J. J. DeLuisi and I. Steutzer, 1967: Comparison of chemiluminescent and Umkehr observations of ozone. *J. Geophys. Res.*, **72**, 1667–1671.

Dave, J. V., 1964: Meaning of successive iteration of the auxiliary equation in the theory of radiative transfer. *Astrophys. J.*, **140**, 1292–1303.

——, 1965: Multiple-scattering in a non-homogeneous, Rayleigh atmosphere. *J. Atmos. Sci.*, **22**, 273–279.

DeLuisi, J. J., 1969: A study of the effect of haze upon Umkehr measurements. *Quart. J. Roy. Meteor. Soc.*, **95**, 181–187.

Dütsch, H. U., 1957: Evaluation of the Umkehr effect by means of a digital electronic computer. Sci. Rept. No. 1, Ozone and general circulation in the stratosphere, Arosa, Lichtklimatisches Observatorium.

——, 1959: Vertical ozone distribution from Umkehr observations. *Arch. Meteor. Geophys. Bioklim.*, **A11**, 240–251.

——, 1966: Two years of regular ozone soundings over Boulder, Colorado. NCAR Tech. Notes, NCAR-TN-10, National Center for Atmospheric Research, Boulder, Colo., 443 pp.

——, and Ch. Ling, 1969: Critical comparison of the determination of vertical ozone distribution by the Umkehr method and by the electrochemical sonde. *Ann. Geophys.*, **25**, 211–214.

Komhyr, W. D., R. G. Grass and R. A. Proulx, 1968: Ozonesonde intercomparison tests. ESSA Res. Labs., Rept. ERL 85-APCL 4, Boulder, Colo. 74 pp.

——, and T. B. Harris, 1965: Note on flow rate measurements made on Mast-Brewer ozone sensor pumps. *Mon. Wea. Rev.*, **93**, 267–268.

Mateer, C. L., 1964: A study of the information content of Umkehr observations. Doctoral dissertation, University of Michigan, 199 pp.

——, 1965: On the information content of Umkehr observations. *J. Atmos. Sci.*, **22**, 370–381.

——, and H. U. Dütsch, 1964: Uniform evaluation of Umkehr observations from the World Ozone Network, Part 1. NCAR, Boulder, Colo., 105 pp.

Pittock, A. B., 1970: On the representativeness of mean ozone distributions. *Quart. J. Roy. Meteor. Soc.*, **96**, 32–39.

Powell, D. B. B., and E. L. Simmons, 1969: Some laboratory and field investigations of the accuracy of Brewer-Mast ozone sensors. *Ann. Geophys.*, **25**, 323–327.

Regener, V. H., 1964: Measurements of atmospheric ozone with the chemiluminescent method. *J. Geophys. Res.*, **69**, 3795–3800.

Rodgers, C. D., 1966: Satellite infrared radiometer—a discussion of inversion methods. University of Oxford, Clarendon Laboratory, Memo. No. 66. 13, 25 pp.

Sekera, Z., and J. V. Dave, 1961: Diffuse transmission of solar ultraviolet radiation in the presence of ozone. *Astrophys. J.*, **133**, 210–227.

Sellers, W. D., and D. N. Yarger, 1969: The statistical prediction of the vertical ozone distribution. *J. Appl. Meteor.*, **8**, 357–361.

Strand, O. N., and E. R. Westwater, 1968: The statistical estimation of the numerical solution of a Fredholm integral equation of the first kind. *J. Assoc. Computing Machinery*, **15**, 104–114.