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APPENDICES

APPENDIX A

The Umkehr raw data collected by the Brewer Control Program and stored in the Ujjjyy.nnn files of the data disk for example of U-file express as below:

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

DDMMYY vt nf AMIN ic C0 0 C0 1 C0 2 C0 3 C0 4 C0 5

301201 343 0 415116 40 357054 409342 436586 471383 499822 507853

DDMMYY vt nf AMIN ic C0 0 C0 1 C0 2 C0 3 C0 4 C0 5

301201 341 0 415155 40 358995 492588 506363 519159 522835 504324

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

where:

DD	=	day
MM	=	month
YY	=	year
vt	=	voltage
nf	=	0/1 (am/pm)
AMIN	=	are minutes to calculate time
ic	=	time conversion
C0 0	=	white noise for first set of measurements, dark count
C0 1	=	counts for first wavelength (306 nm) in the first set of measurements
C0 2	=	counts at 310
C0 3	=	counts at 313
C0 4	=	counts at 317
C0 5	=	counts at 319
C1 0	=	white noise for the second set of measurements
C1 1	=	counts for first wavelength (317 nm) in the second set of measurements
C1 2	=	counts at 319
C1 3	=	counts at 323
C1 4	=	counts at 326
C1 5	=	counts at 329

APPENDIX B

The data are reduced to records of the log (base 10) (times 100) of the light intensity measured at each of the Umkehr wavelengths at the set of standard Umkehr angle. The second step is the Umkehr analysis where the log (base 10) (times 100) of the light intensity to be calculated and give the ozone values in form of ozone profile (in number density and Dobson Unit). The detail of Brewer processing and analysis can be seen as follows:

1. The Preprocessor

The "raw" data collected by the Brewer Control Program and stored in the Ujjjyy.nnn files on the data disk, are reduced to records of the log (base 10) (times 100) of the light intensity measured at each of the Umkehr wavelengths at the set of standard Umkehr angles.

The Ujjjyy.nnn format represents a set of Umkehr measurements made on Julian day number jjj in year yy using instrument number nnn. For example U35701.120 represents an Umkehr observation taken on Julian day 357 in 2001 (December 23, 2001) using instrument number 120 (located at Songkhla). The data read in form the U format files is analyzed using information in the preprocessing setup file and the reduced data is recorded in a disk file for processing by the Umkehr analysis program in a later step.

The preprocessing program is called PREPRO and exists as file PREPRO.EXE on the program disk. It is invoked by a command in the following format:

PREPRO *in data, out list, out data, out graph, debug*

PREPRO U35701.120 UP35701.120 UD35701.120 UG35701.120

Where the various parameters represent the names of input and output data files used or produced by the program, where:

in data is the data collected an Umkehr file by the Brewer Control Program (usual format Ujjjyy.nnn).

out list is the preprocessor output listing (usual format UPjjjyy.nnn).

out data is the data produced by the PREPRO program, and used as input to the Umkehr analysis program (Usual format UDjjjyy.nnn).

out graph is the reduced data in format suitable for graphical presentation (usual format UGjjjyy.nnn).

debug is a non-zero value for this parameter (integer) will cause diagnostic printout to be added to the output listing file out list.

This processing command can be generated by the use of the batch file RUNPRE.BAT by entering:

RUNPRE 35701.120

The preprocessor uses the contents of the file PRESETUP.nnn file which contains a number of parameters needed by the program in order to reduce the Umkehr observations. The file included with the software disk was used to analyses data collected at Songkhla, Thailand. Using this file as a starting point, a new file (with the same name and correct instrument number so that the program can find it) should be prepared which is appropriate for the location for which Umkehr data is to be analyzed. The PRESETUP.120 is:

```
**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****
    ozoavg01.120
    0345  SK   07.200  -100.600
    80.0     89.0
    /*  name of daily ozone file                    */
    /*  station number, header code, latitude and longitude  */
    /*  max_start and max_end angles for rejecting Umkehr    */
**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****
```

The file name ozoavg01.120 is the form of the file name to be used by the preprocessor to find a file with a summary of total ozone for the year the Umkehr data were taken. At the time the program runs it will use the first few characters to define the file name and substitute automatically, the year and instrument number from the U file to be processed. For example ozoavag01.120 would be changed to ozoavag02.121 at run time if an input file name of U20802.121 were specified as input to the preprocessor.

Inside the ozoavg files, the first three entries on each line are the Julian local date (dddyy), the total ozone and the SO_2 column.

The latitude and longitude are to be input in degrees and decimal degrees, and so will be the same values used in the Brewer Control Program.

The preprocessor takes the observation data from the U format file and applies dark count and dead time corrections and scales the light intensities on the 8 Umkehr wavelengths to be in counts per second. The logs (to the base 10) of the light intensity

values calculated from the observations are fitted with a smooth curve using a least squares cubic spline algorithm. The algorithm has points where the spline coefficients are fixed at a number of solar zenith angles (58.0, 63.0, 68.0, 72.0, 76.0, 79.0, 82.0, 85.0, 88.0, and 92.0). From the spline fit, the log intensity values for the "standard Umkehr angles" are interpolated. These values are written out to an output file to serve as input data for the program which calculates the vertical distribution of ozone.

2. The Umkehr Analysis

The Umkehr analysis program is called TOMKEHR.EXE. It can be invoked by entering the command: TOMKEHR *in file, list file, out file, density file, parameter* where:

in file is the filename of data file produced by the PREPRO program (usual format UDjjjyy.nnn).

list file is the output listing file for the Umkehr analysis output (usual format USjjjyy.nnn).

out file is the Umkehr output data in archive format for inclusion in a file which contains many Umkehr-formats (usual format UOjjjyy.nnn).

density file is the file containing a splined, interpolated density height profile which is equivalent to the Umkehr layer output produced by the program (usual format UNjjjyy.nnn)

parameter is a missing (or 0 mean no diagnostic printout, 1 mean diagnostic printout)

In addition to the information read in form the input data file the program also reads in a set of parameter values from the file called UMKSETUP.FIL. This file contains the following:

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

SXUNI4M.DAT
STDTABS.DAT
O3TABLE.DAT
CQMS.DAT
5.974 4.057 2.306 1.548 0.8653
0.6679 0.2733 0.1381 0.07686 .. ozone coefficients for #120 stn SK
6 6 11 12 1 1.0 1000
345 1 7.200 0

0 ... debug file

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

The first four lines contain the names of files which contain data required by the program. The first is the ozone distribution covariance matrix for the layers in the atmosphere which are varied in order to derive a solution. Two covariance matrices are provided; one is an unbiased or uniform matrix called SXUNI4M.DAT and the other is a climatological covariance matrix named SXCLIMAT.DAT.

The file STDTABS.DAT provides a mean atmospheric pressure profile and the file O3TABLE.DAT contains constants which are used by the program to construct a first-guess profile for the inversion process using the analytic expression.

CQMS.DAT is a file containing multiple scattering corrections which are used to correct approximately for the multiple scattered light component included in the Umkehr measurements.

The first line of numbers is values for a number of program parameters. The parameters are KBMIN (the smallest SZA (60, 65, 70, 74, 77, 80, respectively) that will be processed and should be in the range 1,...,6), KBMAX (the largest beginning SZA (83, 85, 86.5, 88, 89 and 90) that will be processed, may also be in the range 1,...,6 but not be less than KBMIN), KEMIN (the lowest value accepted for the last smallest SZA, should be either 11 or 12 (77 or 80)), KEMAX (the highest value accepted for the last largest SZA, should be either 11 or 12 (89 or 90)), JUZPR (printed output which can be turned on by setting JUZPR=1), OMFAC (the total ozone value consistent with the absorption coefficients, used with each Umkehr observation, OMFAC = 1.0 must be used) and SURFACE FRESSURE (in millibars).

The next line contains values for the station ID number, the parameter ILAT (latitude code which should be 1) and JUZTMP (temperature correction code which should be 0). The last line defines the value of the DEBUG parameter, if this value is 0 debugging output is not produced and if it is 1 debugging output is provided.

The TOMKEHR program can be run using a command which looks like the following:

TOMKEHR UD35701.120 US35701.120 UO35701.120 UN35701.120

Alternatively, the command could be generated through the use of the batch file RUNUMK.BAT by entering:

RUNUMK 35701.120

There are several outputs from the TOMKEHR program as indicated earlier. These include the listing file (USjjjyy.nnn), the output data file (UOjjjyy.nnn) and the density height profile (UNjjjyy.nnn). A portion of the listing file for the Songkhla results for December 23, 2001 show below.

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

Date 23 12 1 PM ID Data Obsvd Total Ozone = 0.260 Soln Total Ozone = 0.2601

Iter = 2 RMSRES = 0.6085 DFRMS = 0.001 DNRMS = 0.03

Nobs 101.2 93.5 80.7 70.8 63.5 60.9 58.8

Nres 1.0 0.6 0.4 0.2 0.5 0.2

Nobs 73.1 80.3 77.3 69.9 60.1 53.4 48.3

Nres 1.0 -0.2 -0.9 -0.6 -0.9 -0.9

Nobs 26.2 34.3 37.3 35.4 29.3 22.9 17.5

Nres 0.7 0.6 0.1 0.2 0.0 0.7

O3 [DU] 1.37 3.45 10.38 28.4 57.6 68.3 48.8 12.4 5.7 23.70

F Guess 1.30 3.22 10.84 28.7 53.7 67.2 52.7 13.0 5.8 9.00

Error % 18.5 14.6 9.6 6.9 7.7 10.2 11.6 18.3 19.4 18.3

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

The line labeled "O_3 [DU]" contains the ozone amounts in units of 10^{-5} m for various Umkehr layers with the highest altitude layer on the left and the surface layer to the right. The error estimate is the absolute error estimate based on the results of the solution process and the prior knowledge profile. The numbers RMSRES (root mean square fit between observed Umkehr and Umkehr calculated for the retrieved profile), DFRMS (root mean square change in $\ln(x/x_0)$) and DNRMS (root mean square change in final square bracket term of Rodger's equation) represent the RMS difference between the observed and modeled Umkehrs, the change in the solution between iterations and the RMS change in the forcing vector on the last iteration.

In general, good Umkehr results are obtained when the iterate parameter printed out in the above table has a value of 3 or less. Most really good observing conditions will yield a solution in 2 iterations. The value of RMSRES should be less than 1.0 and preferably less than 0.7.

If an output density-height plot is produced, it will be in the following format. Two columns of data represent a profile of ozone in molecules per cubic centimeter as a function of height kilometers. The first point in the table will be the first even kilometer height above the computed station height (as derived from the standard

atmosphere and the station surface pressure). The output points are calculated for every 2 km, with the top height being 50 km.

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

Date 23 12 1 PM ID Data Obsvd Total Ozone = 0.260 Soln Total Ozone = 0.2601

Iter = 2 RMSRES = 0.6085 DFRMS = 0.001 DNRMS = 0.03

50.00, 5.73E+010, 5.32E+010, 0.078,
48.00, 9.08E+010, 8.32E+010, 0.091,
46.00, 1.45E+011, 1.33E+011, 0.090,
44.00, 2.28E+011, 2.16E+011, 0.060,
42.00, 3.53E+011, 3.53E+011, 0.000,
40.00, 5.43E+011, 5.70E+011, -0.048,
38.00, 8.43E+011, 8.95E+011, -0.058,
36.00, 1.30E+012, 1.35E+012, -0.031,
34.00, 1.95E+012, 1.93E+012, 0.009,
32.00, 2.76E+012, 2.62E+012, 0.053,
30.00, 3.53E+012, 3.26E+012, 0.081,
28.00, 4.02E+012, 3.77E+012, 0.067,
26.00, 4.10E+012, 4.02E+012, 0.019,
24.00, 3.85E+012, 3.97E+012, -0.031,
22.00, 3.28E+012, 3.53E+012, -0.069,
20.00, 2.30E+012, 2.53E+012, -0.092,
18.00, 1.12E+012, 1.20E+012, -0.071,
16.00, 3.96E+011, 3.86E+011, 0.025,
14.00, 2.90E+011, 2.85E+011, 0.018,
12.00, 3.64E+011, 3.76E+011, -0.033,
10.00, 4.30E+011, 4.39E+011, -0.019,
8.00, 4.96E+011, 4.95E+011, 0.002,
6.00, 5.77E+011, 5.71E+011, 0.010,
4.00, 6.71E+011, 6.65E+011, 0.009,
2.00, 7.76E+011, 7.72E+011, 0.005,

Column density from 1.00 km to 51.00 km is 6.89E+018 mol/cm**3

**** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

The Umkehr layer distribution and the density-height plot show two total ozone values. The observed total ozone is the value input via the OZjjjyy.nnn file and the

solution value is the total ozone which the inversion algorithm found to provide the optimum fit to the Umkehr observations. The difference between these values is minimized as one of a number of adjusted values in the process of doing the inversion.

Finally, the UOjjjyy.nnn is written and contains a condensed version of the Umkehr profile which can be conveniently archived along with the results from other analyses. It is in the form:

*** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

260 26012312 1 2 137 345 1038 284 576 683 488 124 57 237

2 511 1 3 61345

*** **** **** **** **** **** **** **** **** **** **** **** **** **** ****

where:

260	is observed total ozone * 1000
2601	is solution total ozone * 10000
23121	is ddmmyy
2	is AM/PM (1=AM, 2 = PM)
137...237	is the top layer to the surface layer of Umkehr distribution
2	is iteration count
5	is starting angle number for Umkehr
11	is last angle in Umkehr
1	is DFRMS * 1000
3	is DNRMS * 1000
61	is RMSRES * 100
345	is station ID number

VITAE

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