

ReadMe instructions on how to run the O3BUmkehr.exe file

O3BUmkehr is the PC based version of the Umkehr retrieval designed for the Brewer Umkehr measurements. The algorithm was originally developed for the Dobson Umkehr version (Petropavlovskikh et al. 2005). It was later (~2005) modified for the Brewer Umkehr measurements taken at ~310 and ~323 nm wavelength channels only. The Brewer Umkehr readings are typically performed at 5 slits, where slit # 2 reads radiation that is transmitted through a band-pass centered at ~310 nm (each instrument has its own spectral settings). The consequent set of Umkehr measurements is taken in most of the Brewer instruments (except the very early versions), where photon count readings are shifted to longer wavelengths by a spectral mask. This algorithm uses the Brewer Umkehr measurements from the second set of readings taken at the slit # 4, which is centered at ~ 326 nm wavelength. The measurements from two selected channels form so-called single-pair N-value that is used for the ozone profile retrieval. Therefore, the algorithm was modified to account for a different set of wavelengths as compared to Dobson. The new set of absorption cross-sections (based on the Bass- and Paur dataset), instrument band-passes (truncated triangular shape), multiple scattering and refraction correction tables, and Jacobians had been created to fit optical parameters of a Brewer instrument. Currently, the measurement error matrix is assumed to be half of what is used for Dobson measurements, which means the reduced level of the measured noise. This value can be altered in the set up of the software (see further).

The software was developed by Martin Stanek from Czech Hydrometeorological Institute, Czech Republic (stanek@chmi.cz). It is still in the test stage, so use it at your own risk.

It is possible to run executable from the command line with two parameters specifying the dates. First parameter is the date and the second parameter is the name of the output file. The date format has to be in the "short format" that is specific for each computer. Martin is using "d.m.yyyy", for example "1.11.2007" and in US it could be "dd/mm/yy" "01/11/07" (needs to be checked for each personal computer).

In the batch file the following line could be used to run code on the daily basis:
O3BUmkehr.exe 1.11.2007 output.txt

Set up

In order to begin using the **O3BUmkehr** software, you will have to set parameters for the station's instrument/computer. This is done by adjusting the input information in the **O3BUmkehr.ini** file. It can be done by opening the file into the user's preferred text editor, changing set up parameters, and saving the file in the same directory as the O3BUmkehr.exe file. It can be also done interactively from the **Setup** window of the

O3BUmkehr software. In order to do it, use the executable file to initiate the software. In the new window select **Setup** tab from the upper panel of the software.

The Setup window contains the following fields and options:

- Instrument number: 184
- Station number: 96
- Input Data Path: \\brewer\b184\bdata\
- Output Data Path: F:\Data\Umkehr\
- Spline Interpolation of N-Values
- 16 Layer Output
- Max. iterations: 5
- 320 Ratio: Quality Filter
- Range: 0.008
- Offset: 0.002
- Wavelength [A.U.] short, long: B-file, 3100.400, 3265.110
- Wavelength - 310, 326 nm: -0.076, -8.350
- Brewer temp. circuit: Old, New
- Total Ozone: Recalculate Total Ozone, Standard Lamp R6: 1855, Weighting const.: 3
- Observation Error: 0.16, 0.18, 0.20, 0.22, 0.25, 0.27, 0.29, 0.30, 0.40, 0.60, 0.80
- Export: Profiles, Observed N - Values
- SZA Range: k begin min: 1, k end min: 11, k begin max: 5, k end max: 12

Figure 1. Set up window

The new **Setup** window will open (see Figure 1). It has a set of parameters that the user can change by typing the new information in white fields for a corresponding parameter. Begin with providing your instrument number (for example, 184) and the number for the operating station (e.g. 96). Then, continue with the change of the directory name for the input (<\\brewer\b184\bdata\>) and output of the retrieved data (F:\Data\Umkehr\).

The user can choose to check the box for the “Spline Interpolation of N-values” option. In this case the interpolation will be used to obtain Umkehr N-values at the nominal SZAs.

The output can be also saved in 16 layers instead of traditional 10. The layer 1 of the 16-layer profile output is situated between the surface and 500 mb, every adjacent layer above it has its top pressure at half of the bottom pressure, where the top layer 16 provides ozone column integrated above ~0.016 mb atmospheric pressure level. The 10 Umkehr layers are formed from the 16 layer profile by combining layers 1 and 2 into the Umkehr layer 1, and by combining layers 11 through 16 into Umkehr layer 10, while other Umkehr layers are single layers linked to the n+1 numbers of the 16-layer profile system, such that Umkehr layer 2 is the same as layer 3 in the 16-layer profile output.

The limit of the iterations can be adjusted in the “Max iterations” box. Typically, a “good” retrieval requires less than 3 iterations.

Another option is to activate the data quality filter option (the box below the “Interpolation” box under the header “320 Ratio”) prior to the interpolation. The current filter is a ratio between two consecutive Umkehr measurements at 320 nm channel, but optimized for Martin’s MKII (Ratio 320 range). The quality filter is designed to eliminate “cloudy” points that fall outside of the error envelop, which can be defined in the “Range” and “Offset” boxes on the right side of the “Quality Filter” box (the default is set to 0.2). The way to define the best quality parameters for your own instrument is to pick a very clear day for measurements, and then open the “Raw data” tab at the top of the main window (you can see it after the set up window is complete and closed). The 320 nm ratio will be plotted as function of the SZA. You can then define the range of the natural variability in your measurement (“Range”) and the mean offset (“Offset”) parameters for you set up window. Click on the “Setup” tab at the top pf the main window and change parameters, then close/save the setup. You might need to check measurements at several clear days to figure out the bets adjustment for the instrument. The cloud clearing method is still under development and could be further modified in the nearest future.

The set up file has an option to use Brewer temperature circuit for the old and new instruments.

The “Wavelength [AU] short, long” boxes are designed to set the center of the wavelengths channels used for the ozone retrieval. It can be adjusted to fit optical characteristics of each instrument. The information on wavelength band-pass and its center can be found in the LF* file which is created by the PO command, or taken from the instrument constants file and the dispersion test. There is a button next to the wavelength set up boxes (short and long wavelength channels) that “recalculates the slit constants”. If chosen, the instrument band-pass functions are aligned to match the center of the instrument specific optical channel. The shape of the band-pass function is kept fixed for all instruments. Next, the band-pass function (wavelengths are registered in the air) is shifted to the wavelengths registered in the vacuum (http://www.kayelaby.npl.co.uk/general_physics/2_5/2_5_7.html). The adjustment is done according to the station’s atmospheric temperature and pressure, whereas these parameters are specified in the **O3BUmkehr.ini** file, for example:

```
Station_Pressure=980      [hPa]
Station_Temperature=15   [C].
```

The final adjustment to the band-pass function is done by interpolating it to the wavelength grid of the spectroscopic coefficients file (ozone and Rayleigh coefficients).

The “Wavelength -310, 326 nm temperature coefficient” boxes can be used to adjust the temperature coefficients at 310 and 326 nm channels that are specific for each instrument (boxes on the right side). The raw counts from the B-file are corrected based on the temperature of the instrument. The temperature correction is programmed in the O3BUmkehr software.

```
version=2
dh
04
01
07
Ft Peck
  48.308
  105.102
  2.29
pr
950
inst
  0
  -.2185
  -.8645
  -1.4434
  -2.3825
```

Figure 2. Example of the B-file for a brewer at the Fort Peck, IL site of the NEUBrew network. The temperature coefficients at 5 channels are highlighted.

The Brewer manual instructs how to compensate readings for instrument internal temperature variability. The count rates F are corrected for the temperature-dependent band-pass characteristics of various filters inside the spectrometer assembly:

$$F \leftarrow F + (PC + TC_i) \cdot TE + AF_i, i = 2..6$$

where

PC is the constant part of the temperature coefficient

TC_i are the wavelength-dependent temperature coefficients read from the spectrophotometer's Constants File (stored on disk)

TE is the instrument temperature in degrees Celsius

AF_i is the attenuation value of the neutral-density filters at position i (the array AF of attenuation values is also read from the instrument Constants File).

However, the neutral density filter is not used in Umkehr measurements, and thus the AF_i is not used for temperature corrections of zenith sky counts. The instrumental temperature coefficients can be calculated from the standard lamp test results (SL test file, ICFJJYY.nnn), or taken from the B-file (Figure 2). The coefficients are referenced against the measurements at the slit #1 (which is set to zero). Temperature coefficients for the 5 shorter channels are recorded in the header of b-file. Typically, the SL test is not performed at the longer wavelength channel (326 nm) that is used in the retrieval.

Therefore, the temperature coefficient at the longer wavelength (O3Tc6 in the *.ini file) has to be extrapolated from shorter wavelengths, while it is not a preferred method. In

order to estimate the temperature coefficients for the longer set of channels the third degree polynomial is fitted to the coefficients measured at the shorter channels:

$$TC = A + B*\lambda + C*\lambda^2 + D*\lambda^3$$

In addition, the 320 nm channel has the same temperature correction for short and long set of wavelengths.

Total ozone (read from the B-file) can be corrected (check in the box “Recalculate Total Ozone”) based on the R6/R5 calibration parameter that can be inserted in the “Standard Lamp R6” box. This information can be found in the calibration report (under “Final SL ratios: R6/R5” header) typically prepared by Ken Lamb from the Ozone International Company after site calibration visit. The ICF file name also can be inserted in the Instrument Constant File box while the corresponding ICF file should be placed in the same directory as the B-file. The “Weighting const” box can be adjusted to give different weight to the R6 value.

The “Observation Errors” are values used in the error covariance matrix. They are provided at 12 nominal SZAs used in the retrieval: 60, 65, 70, 74, 77, 80, 83, 85, 86.5, 88, 89, and 90 degrees (0.16 value at 60 SZA is shown in Figure 1). The default values had been adapted from the Dobson retrieval algorithm. The measurement errors for the Dobson Umkehr retrieval were derived based on long-term comparisons between two Dobsons (#101 and #051) that were operated side-by-side at Arosa station in Switzerland between 1988 and 1999 (note, only 1994-1999 period was chosen for comparisons to avoid intermittent shifts between instruments). However, for the Brewer retrievals the measurement errors were set to the half of the Dobson errors. The assumption is that the typical Brewer measurements are less noisy (better signal to noise ratio), than the typical Dobson measurements. It may be true for Brewer Mark II and III instruments, but not for Mark IV. Recent comparisons of two Mark IV instruments (#141 and # 134), which were operated under NEUBrew network in Boulder, CO between 2006 and 2009, show that the relative noise (RMSD) in co-incident measurements is similar to previously defined Dobson measurement noise.

For the export of files, the user can choose between profiles or N-values. It will create the output file that will be saved in the output directory.

The set of parameters under the ”SZA range” boxes is also available to define the SZA range. The numbers 1 though 12 correspond to the 12 nominal SZAs defined above. The beginning of the Umkehr measurement (the highest sun elevation) and the end (the lowest sun elevation) can be restricted by these parameters. Figure 1 shows that in order to retrieve ozone profile, the morning or afternoon Umkehr measurements has to cover SZA range between at least 77 (K begin max = 5) and 89 degrees (K end min = 11).

Upon finishing with the set up window, choose the OK button to save new settings. The new setting choices will be automatically saved in the O3BUmkehr.ini file.

Reading in data

The algorithm uses B-files for reading in daily Umkehr measurements, along with total ozone information and temperature of the instrument. The total ozone average is calculated for the morning and afternoon separately. It is weighted to be more representative for morning and evening.

The data file can be read in by using the "Read B file" tab at the top of the software window and choosing the file from the pop up browser window. Another option is to choose the date from the pool down calendar menu at the top left corner. The software will find the B-file for the selected date and will activate the retrieval. If the date is not available, the software will be not activated. At the top of the window there is a Data Export tab where the long-term measurement period can be chosen from the pop-up menu. There is also a set up option for automated rejection of retrieved data based on selected number of iterations (usually less than 4) and residual of the retrieval (less than 10) . In this case, the Umkehr ozone profile retrieval results for multiple days will be saved in the file, that has to be specified in the pop-up browser window that appears once the OK button is hit.

In the O3BUmkehr.ini file the user can adjust ozone absorption cross sections to match the station's instrument specific parameters (adjust the center of the channel for short and long wavelengths). The information about the center of the channel and an effective ozone absorption coefficients (based on convolution of the Bass and Paur spectroscopic dataset and band-pass, for stratospheric temperature set at -44 C) can be found in the Umksetup file or lfjjjyy.nnn (the end of the output from dispersion test processing). However, the retrieval algorithm does not utilize these coefficients, but instead uses convolution of the spectrally resolved radiances with the band-pass and the extra-terrestrial solar flux data to simulate Umkehr measurements (see more in Petropavlovskikh et al, 2005).

Retrieval information

On the left side of the window you will have some information regarding how successful your retrieval is. The "good" retrieval means less than 3 iterations were required, and the following three numbers (RMSD of the residuals in RT) should be less than 1.00

RMSres is the root-mean squar deviation (RMSD) of the difference from the solution from the previous iteration

DFRMS the the RMSD of the convergency of the forcing factor

NDRMS is the the RMSD of the residual fit (difference between OB and RT N-values)

The "bad" retrieval is when statistics did not meet requirements of convergence or profile has negative data.

The two tabs allow you to view results in graphs (N-values and ozone profiles for morning and afternoon measuremnets) or as summary of Results. The retrieved ozone is called TDXN and is given in 10 layers, beginning from layer 10, 9..., last layer is double layer 0+1.

I do not have any written guide for this software yet. The results can be **saved** as **1) N-values at 14 nominal SZAs** (chosed the “Save N-value” tab shows when N-values are viewed as graph, choose from upper tab)

```
1 Boulder 40.13 830.0
12 01 2007 1 3 4 11 0 321 -1.0 -1.0 -1.0 68.7 82.8 99.7 112.9 116.2 113.9 109.2
105.7 -1.0 1
```

date(DD/MM/YYYY), morning/afternoon (1/2), wavelength pair (3), First available SZA (4), last available SZA(11), clear sky (0), total ozone (321), 12 N-values (fitted with spline in observed points, N-value is $100 \cdot \log_{10}(I_{232}/I_{310})$, missing values are marked as -1), station #.

2) **all measured N-values** (when saving the option 1, all measured N-values at 306, 310, 313, 317, 320, 323, 326 and 329 nm are automatically saved under names such as N306_*, N310_*, N313_*, N317_*, N320_*, N323_8, N326_*, or N329_* with extension "date.num" files, where "date" is written as julyy, or julian day and year, and num is three digit station number. Files are saved in the output directory only as specified in the *.ini file). Example:

```
9/26/2007 12:56:01 PM 90.04 367.68920
9/26/2007 12:59:26 PM 89.39 382.00249
9/26/2007 1:02:03 PM 88.89 391.26228
9/26/2007 1:04:40 PM 88.39 399.70918
9/26/2007 1:07:17 PM 87.89 407.71787
```

3) **ozone profiles** (choose to view ozone profiles, then you will be given an option to save results in the file) under following format:

date, observe and solution TO, iterations, statistics, column density
observed N-values,
a prioir,
solution in DU,
height in km
density profile interpolated to a nominal height

```
1/12/2007 AM Boulder
OBS TOZ 320.7 SOL TOZ 320.7 ITER 3 RES 0.414 DF 0.003 DN 0.010 COL
DENSITY 8.50123092231121E+0018
INITL NVAL 68.7 82.8 99.7 112.9 116.2 113.9 109.2 105.7
A PRIORI PROF (DU) 1.67 3.95 10.64 20.96 37.77 66.04 78.68 52.36 29.76 21.78
SOLUTION PROF (DU) 1.78 4.40 11.87 23.95 48.25 81.54 73.31 37.17 20.37 18.06
HEIGHT 50.00 48.00 46.00 44.00 42.00 40.00 38.00 36.00 34.00 32.00
30.00 28.00 26.00 24.00 22.00 20.00 18.00 16.00 14.00 12.00 10.00 8.00
6.00 4.00 2.00
DENSITY 0.71 1.12 1.80 2.83 4.28 6.17 8.53 11.34 15.23 21.08
29.10 39.16 48.90 52.97 48.13 38.38 27.24 18.87 14.90 11.58 7.70 5.13
4.52 5.41 0.00
```

4) Summary file

Results of the retrieval can be saved in the summary file. Click on the tab “Results” at the top of the viewing windows choices. User can either print the page or save it in the file.

The following format is self-explanatory:

L means lower wavelength channel at 310 nm

H is higher channel at 326 nm

VNOB are observed N-values after the least-square fit to the nominal SZAs. Only N-values at measured SZAs are displayed, where kb and ke are 1 through 12 number that indicate range of available nominal SZAs: 60, 65, 70, 74, 77, 80, 83, 85, 86.5, 88, 89, and 90 degrees. No SZA extrapolation is allowed.

FRES is the residuals between the observed and retrieved profile associated N-values

TDXN is the retrieved ozone profile in 10 layers.

The AK is available in 8 layers –rows of the AK represent weighting of the observed profiles into individual layer: 9+, 8, 7, 6, 5, 4, 3+2, and 0+1.

The last segment is the table of ozone concentration given as function of altitude. The altitude is estimated from standard pressure of Umkehr layers using the “phprofil.dat” file that contains the US standard atmosphere pressure profile as function of altitude. The concentration of Umkehr layer ozone is derived by multiplying DU by Lods Schmidt number ($P_0/k/T_0=2.687 \cdot 10^{19}$ particles/cm³) and dividing it by 2 (per 2 km resolution).

For included example (shown below) the column density integrated between 1.00 km and 51.00 km altitude turned out to be $7.64259418647139E+0018$ molecules/cm³. The Umkehr number density is interpolated to vertical profile at 2 km resolution.

```

*** Umkehr Ozone Profile ***
Date: 7/8/2007 PM Brewer #171 TableMountain Latitude: 34.38 Surface
Pressure: 760

Observed N-Values
SZA 0.00 0.00 0.00 0.00 0.00 0.00 83.00 85.00 86.50 88.00 89.00
90.00
L 0.00 0.00 0.00 0.00 0.00 0.00 427.94 406.67 391.99 376.80 364.84
351.49
H 0.00 0.00 0.00 0.00 0.00 0.00 599.85 583.03 566.52 545.31 527.62
506.38
H-L 0.00 0.00 0.00 0.00 0.00 0.00 171.91 176.36 174.52 168.52 162.78
154.88

AP Profile
0.11 0.34 0.97 2.89 9.56 26.16 53.01 74.68 63.71 28.90 14.81 14.73
12.39
INITL NRES
36.99 36.69 36.06 35.34 35.20 34.42

*** Result ***
Obsvd Total Ozone = 0.2889
Soln Total Ozone = 0.2895
Iter = 2 RMSRES = 0.1409 DFRMS = 0.016 NDRMS = 0.01

kb = 7 ke = 12
VNOB 171.87 176.29 174.41 168.36 162.57 154.60
FRES -38.87 -38.96 -38.80 -38.77 -39.11 -38.69
TDXN 1.34 2.60 8.43 24.50 53.66 74.80 59.80 26.21 13.38
24.82

8-layer averaging kernel
0.992 0.009 -0.003 0.001 -0.001 0.002 -0.002 0.001
0.164 0.843 0.059 -0.040 0.032 -0.018 -0.002 0.006
-0.134 0.168 0.959 -0.004 -0.017 0.052 -0.075 0.058
0.784 -0.585 0.318 0.642 0.210 0.062 -0.354 0.333
-1.552 1.453 -0.584 0.482 0.555 0.306 0.046 -0.230

```



```

0.546  -0.690   0.175  -0.049   0.244   0.485   0.578  -0.321
0.143  -0.007   0.082  -0.156   0.033   0.186   0.597   0.352
0.023  -0.075  -0.014   0.076  -0.044  -0.049   0.241   0.705

```

```

50.00  4.97135155080264E+0010
48.00  7.15131020190814E+0010
46.00  1.06907745030990E+0011
44.00  1.64581655307368E+0011
42.00  2.63929424431830E+0011
40.00  4.25537228013428E+0011
38.00  6.83826174122280E+0011
36.00  1.07606559988033E+0012
34.00  1.64620618724744E+0012
32.00  2.39937058693783E+0012
30.00  3.26565241376548E+0012
28.00  4.05966842223165E+0012
26.00  4.52648185521067E+0012
24.00  4.51655032512857E+0012
22.00  3.96912680369849E+0012
20.00  3.05016697009573E+0012
18.00  2.01426382360625E+0012
16.00  1.24816267744450E+0012
14.00  9.02635458169623E+0011
12.00  7.69486290451257E+0011
10.00  7.42220540780966E+0011
8.00   7.48084430095212E+0011
6.00   7.51342373665920E+0011
4.00   7.61477329514021E+0011

```

Column density from 1.00 km to 51.00 km is 7.64259418647139E+0018 molecules/cm³

5) TESTAK.dat file

In the “graph” window’s upper panel there is an option for saving the averaging kernel for each successful ozone profile retrieval. The file contains the Averaging Kernel coefficients for 16 Umkehr layers (top to bottom).

The file also includes the 16-layer AP ozone profile required for calculations of the smoothed ozone profiles:

$X_{sm}(j) = \sum_k AK(k,j) * (X_{true}(k) - AP(k)) + AP(j)$, where X_{sm} is the smoothed ozone profile, X_{true} is the compared ozone profile (for example, the ozone sounding profile can be integrated in Umkehr layers up to the balloon burst pressure level and AP profile information used in layers above that), the AP is the a priori ozone profile, \sum_k represents the integral of the AK weighted ozone residuals in all $k=1,16$ layers.

Printing out the Averaging Kernels

```

1/1/2008  AM  dsrc  Total Ozone: 0.305
-0.000004  0.066775  0.015919  0.003852  -0.000625  -
0.000026  0.000034  0.000010  0.000003  0.000001  -
0.000002  -0.000001  0.000001  -0.000004  0.000013  -
0.000001
-0.000017  0.290784  0.069324  0.016773  -0.002720  -
0.000113  0.000148  0.000043  0.000012  0.000005  -
0.000010  -0.000004  0.000003  -0.000017  0.000059  -
0.000005
-0.000103  1.181813  0.305692  0.080946  -0.008556
0.000566  0.000773  0.000155  0.000040  -0.000010  -
0.000030  -0.000004  0.000005  -0.000114  0.000282  -
0.000025

```

-0.000485	3.261235	0.949912	0.279467	0.025855				
0.011606	0.002667	0.000299	0.000067	-0.000134	-			
0.000051	0.000043	-0.000011	-0.000546	0.001064	-			
0.000091								
-0.000471	0.275942	-0.126353	-0.161299	0.818132				
0.090268	-0.012663	0.003433	0.000008	-0.000065	-			
0.000192	-0.000085	0.000116	-0.000551	0.001253				
0.000154								
0.002971	-3.673195	0.162349	0.656369	1.005909				
0.420954	0.107289	-0.015448	-0.003025	0.002215	-			
0.000310	0.000550	0.000070	0.002426	-0.007392				
0.000989								
0.021102	43.662599	13.531180	5.095824	-1.149576				
0.970245	0.534085	0.018267	-0.012690	0.003175				
0.005194	0.000996	-0.001009	0.021783	-0.051354				
0.001610								
0.055946	272.383040	40.886353	-3.314270	4.335002	-			
1.035830	-0.113003	0.739892	0.067410	-0.043907				
0.042932	-0.007393	-0.009722	0.078005	-0.146312	-			
0.005365								
0.102074	604.641352	50.686083	-14.785854	6.753299	-			
1.274793	-0.844627	0.206401	0.760922	0.112352	-			
0.032890	0.034563	0.002136	0.063160	-0.238784				
0.029498								
0.064763	762.371783	-4.728827	-35.222901	2.961222				
1.149457	0.228955	-0.650554	0.337832	0.795169				
0.129500	-0.054722	-0.013022	0.094776	-0.026356	-			
0.108529								
-0.185056	-831.570921	-58.819115	26.379923	-4.887214	-			
1.327023	0.068053	1.131790	-0.572971	0.366145				
0.722659	0.164019	-0.070262	-0.211461	0.430574	-			
0.093380								
0.357876	-1228.467932	-31.279408	56.885245	-13.236252				
1.923968	0.847454	-0.301033	0.356494	-0.231648				
0.220361	0.643135	0.526313	-0.263897	-0.295031				
0.402836								
-0.150758	-68.587318	-15.631578	-6.186663	-0.397763				
0.423148	0.295445	-0.132252	0.104435	-0.035781	-			
0.047890	0.171238	0.509454	0.581592	-0.013128	-			
0.276584								
-0.104154	169.059764	-9.768480	-15.029221	1.857161	-			
0.148475	0.026923	0.061495	-0.033801	0.021386	-			
0.014189	-0.020963	0.174308	0.555480	0.461347	-			
0.074218								
0.065645	150.966411	22.072055	2.658621	1.242677	-			
0.284467	-0.263317	-0.028686	-0.029929	0.007878				
0.015918	-0.009804	-0.013650	0.175651	0.570676				
0.217405								
0.228714	99.720455	14.022339	0.436544	1.147332	-			
0.126450	-0.174069	-0.043062	0.000330	-0.004979				
0.003877	0.017707	-0.049330	0.048311	0.440948				
0.371239								
AP Profile								
0.001	0.004	0.017	0.079	0.359	1.087	3.519	10.472	22.630
41.811	67.711	70.431	37.029	20.467	11.726	10.170		

AM and PM TO calculation

For the Umkehr retrieval, the TO is based on all “good” DS (direct sun-light measurements) taken in the morning or in the afternoon, where the “good” DS would have standard deviation less than 2, and the Brewer instrument Temperature is not -30. There is no ZS (Zenith sky) results included. The AM/PM TO is calculated using the asymmetrical Gauss filter:

$$f_x = 1 / (\text{Weighting_constant} * \text{SQRT}(2 * \text{PI})) * \text{EXP}(- dt^2 / (2 * \text{Weighting_constant}^2))$$

The Weighting_constant can have 1 to 10 number in Setup, dt is the time shift that represents how "old" is the value: 0..10 can be used if 11 DS measurements are available in AM or PM.

This result should be more representative than the simple AVG, if TO goes up or down during the day. If the averaging AVG is preferred the Weighting_constant should be set to 10, with Weighting_constant 1 about (not exactly) the first AM DS or last PM DS will be used. Currently, the Weighting_constant is set to 3 5.

The O3 value can be manually overwritten on the main screen of the program and activated in the check box in order to recalculate profile.

Applying the standard lamp correction.

The standard lamp (SL) is placed at the beginning of the optical part in the Brewer. The double ratios R5 and R6 are calculated the same way, like from the sun light during DS TO measurements. It is assumed that these ratios are stable. These assumptions remain valid even when the intensity of SL lamp decreases, until it remains above a critical value (reference to Martin). At the same time, the voltage of the lamp must be stable too. If the SL is stable, all changes of the calculated R5/R6 from this lamp reflect the changes in the optics or photomultiplier. Then, the change in R6 ratio can be used to correct the ETC constant.

For example, B#141 has 2075/3860 SL (numbers are taken from “Final SL ratio: R6/R5” in the Ken Lamb calibration report).

The Final ETC constants for Boulder are 3232/3390 as recorded in the ICF23306.141 file (line 10/11).

There are three SL tests recorded in the b-file B00108.141. The average R6/R5 SL ratio is 2081/3899. It means that the difference from the report is 6/39. Because there is an increase in the SL ratios, the ETC constants (both O3 -> R6 and SO2 -> R5 in this case) should be increased to 3232+6 and 3390+39 respectively.

In this example SL-R6_Ref_Reading (r6) is 2075. The O3BUmkehr can calculate ETC correction based on this number (2075) and recalculate TO using new ETC.

It is possible to still have the same ratio after the lamp replacement. If not, the new reference should be used, but the old SL corrections have to be taken into account too.

There is no need to use ICF for TO recalculation because all necessary constants are saved in the b-file (lines 22 and 23 contain Final ETC constants that are copied in the b-file from the recent calibration ICF file). However, the availability of the ICF files will

give a chance to use new (better) constants like TCs, dead time, absorption ... There is an option in the O3BUmkehr setup to use ICF file to update the external constants.

Some equations and ozone conversions

If I use the equation $dP = -\rho * g * dZ$, where ρ is density of air (g/cm^3), g is acceleration constant ($9.81 \text{ m}/\text{s}^2$) and dP is pressure difference ($10^5 \text{ g} * \text{m}/\text{s}^2 / \text{cm}^2 / 10^6$). Then the integrated air density * 1 km is about $10.3 \text{ g} * \text{km}/\text{cm}^3$. The DU (10^{-3} atm cm) is converted to particles/ cm^2 by Loschmidt number ($P_0/k/T_0 = 2.687 \cdot 10^{19}$ particles/ cm^3).

Integrated Air density ($10.3 \cdot 10^3 \text{ g} * \text{cm}/\text{cm}^3$) / M ($28.996 \text{ g}/\text{mole}$) * N_a ($6.0225 \cdot 10^{23}$ particle/mole) = $2.15 \cdot 10^{26}$ (particle/ cm^2).

To calculate the ozone column density – interpolate Umkehr layer ozone on 1 km grid using standard pressure/altitude file for interpolation (use log(partial column ozone) vs log (pressure) for interpolation), and follow three yellow highlighted equations and integrate ozone density profile. For temperature profile use values either calculated from hydro-static equation ($dP/P = -\rho * g * dz$), or use climatological temperature profile available from Umkehr code:

Ozone Partial Pressure (nb)

$$P_{O_3} = 0.55 * O_3(DU) / \log_{10}(P_{\text{btm}}/P_{\text{top}}) \quad (\text{mbar})$$

mb = millibar

nb = nanobar (10^{-9} bar) = 10^{-4} Pa

h Pa = hecto pascal

where 0.55 is

$$L * g * \mu(\text{air}) / N_a / \ln(10) = 2.687 \cdot 10^{19} * 9.8 * 28.996 / 6.0225 \cdot 10^{23} / 2.3 = 0.55 \text{ (mb)}$$

Loschmidt number $L = P_0/k/T_0 = 2.687 \cdot 10^{19}$ (particles/ cm^3)

Acceleration constant $g = 9.8$ (m/s²)

Mole mass of air $\mu(\text{air}) = 28.996$ (g/mole)

Ozone amount O_3 (DU or 0.01 atm cm)

Ozone Mass Density $D_{O_3} = P_{O_3} / (1732220 * T)$ (kg/m³)

Where $173.2220 \text{ (Pa} * \text{m}^3/\text{K}/\text{kg}) = R / \mu(O_3) = 8.314427 / 48 * 10^{-3} = 1732180 \text{ (nb} * \text{m}^3/\text{K}/\text{kg})$

Mole mass of ozone $M(O_3) = 48$ (g/mole)

Avogadro number $N_a = 6.0225 \cdot 10^{23}$ (particle/mole)

Boltzmann constant $K = 1.3806504(24) \times 10^{-23}$ (J/K)

Gas constant $R = N_a * K = 8.314472$ (J/mole/K = $\text{Pa} * \text{m}^3/\text{mole}/\text{K} = \text{kg} * \text{m}^2/\text{s}^2/\text{mole}/\text{K}$)

$$1 \text{ J} = 1 \text{ kg m}^2/\text{s}^2$$

$$1 \text{ mb} = 10^{-3} \text{ bar} = 100 \text{ Pa} = 100 \text{ kg}/\text{m} * \text{s}^2$$

$$1 \text{ Pa} = 1 \text{ N}/\text{m}^2 = 10^4 \text{ nb}$$

$$1 \text{ N} = 1 \text{ kg} * \text{m}/\text{s}^2$$

$$1 \text{ J} = 1 \text{ Pa} * \text{m}^3$$

Ozone Number Density $n = 1.25467 \cdot 10^{19} * D_{O_3}$ (molecules/cm³)

Where $1.25467 * 10^{19} = N_a / \mu(O_3)$ (particle/g)

Ozone Column Density $E = 46696.8 * D_{O_3}$ (atoms-cm/km)

$$\text{Air Density} \quad D_{\text{air}} = P / (2.87053 * T) \quad (\text{kg/m}^3)$$

Molar concentration

For any substance, the number density n (in units of m^{-3}) can be expressed in terms of its molar concentration c (in units of mole/m^3) as:

$$n = N_A c,$$

where N_A is the Avogadro constant $\approx 6.022 \times 10^{23} \text{ mol}^{-1}$. This is still true if the spatial dimension unit, meter, in both n and c is consistently replaced by any other spatial dimension unit, e.g. if n is in units of cm^{-3} and c is in units of mole/cm^3 , or if n is in units of L^{-1} and c is in units of mole/L , etc.

Mass density

For atoms or molecules of a well-defined molecular mass M (in units of kg/mole), the number density can be expressed in terms of the mass density of a substance ρ (in units of kg/m^3) as

$$n = N_A / M * \rho .$$

Note that the ratio M/N_A is the mass of a single atom or molecule in units of kg .

Details of calculation of the ozone column number density

$$P_{O_3} = L * g * \mu(O_3) * O_3(\text{DU}) / N_A / \log_{10}(P_1/P_2) / \ln(10)$$

$$D_{O_3} = P_{O_3} / (1732220 * T) = L * g * \mu(O_3) * O_3(\text{DU}) / N_A / \log_{10}(P_1/P_2) / \ln(10) * \mu(O_3) / R / T$$

$$n = 12546700000000000000 * D_{O_3} = \frac{N_A / \mu(O_3) * L * g * \mu(\text{air}) * O_3(\text{DU})}{N_A / \log_{10}(P_1/P_2) / \ln(10) * \mu(O_3) / R / T} \quad (\text{equation A}),$$

where yellow highlights indicate values that cancel out

Then, using Ideal gas law $P = \rho * R * T / \mu(\text{air})$
 and hydrostatic equation $dP = - \rho * g * dz$,
 from which $\rho = - dP/g/dz$, and substituting it to Ideal gas law we get:
 $P = dP * R * T / \mu(\text{air}) / g / dz$

Re-arranging parameters of the above equation, we get $\mu(\text{air}) * g / R / T = - dP/P / dz = \ln(P_1/P_2) / (z_2 - z_1)$ and substitute parameters in our equation (A) that are highlighted in red color, such that
 $n = L * O_3(\text{DU}) * \ln(P_1/P_2) / \log_{10}(P_1/P_2) / \ln(10) / (Z_2 - Z_1)$,
 where Z_2 and Z_1 are altitude (km) of the top and bottom of the ozone layer.
 While using conversion of $\ln(P) = \log_{10}(P) * \ln(10)$, we get the $\ln(P_1/P_2) * \ln(10)$ canceled out.
 Thus, $n = L * O_3(\text{DU}) / (Z_2 - Z_1) * 10^8$, where 10^8 is conversion from cm to km