ACE-MAESTRO Level 2 Version 3.12 Beta Data Description and File Formats

ACE-MAESTRO Team

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	Function	Name	Signature	Date
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Document change record

Issue	Revision	Date	Comments
1	A	2013/03/26	Initial Document
	B	2013/04/15	Data access is generally via web-based download rather than sftp

1. Introduction of MAESTRO level 2 version 3.12 beta data

The MAESTRO level 2 version 3.12 beta data is the latest release after the operational v1.2 data. The new data is at the beta stage and is not validated.

One persistent problem in developing the MAESTRO retrieval algorithms is the lack of an accurate time stamp for the MAESTRO measurement relative to the FTS time. The MAESTRO retrieval uses the ACE-FTS derived atmospheric data that contains the time, tangent height, pressure and temperature as the reference. The MAESTRO instrument time stamp is not consistent with the FTS time stamp. A time correction has to be introduced in order to obtain accurate tangent altitudes to use in the profile retrievals. In MAESTRO v1.2 the MAESTRO and FTS time difference was set fixed and was determined by finding the best match between the MAESTRO and FTS ozone profiles for a one year data set. The MAESTRO v1.2 mixing ratio profiles agree with FTS reasonably well except for some distinct discrepancies at high UTC times when satellite command uploads take place. It is suggested that the interrupt latency in the satellite bus computer has been the cause of the timing problem [1].

The current MAESTRO v3.12 algorithm determines the MAESTRO and FTS time difference for each occultation measurement by searching the best fit of MAESTRO O_2 A- or B- band slant column amounts to the air mass slant column amounts derived from the FTS v3.0 pressure and temperature data. The sunrise and sunset were treated separately and adopted different values for the O_2 to air column scaling factor.

The MAESTRO v3.12 beta data consists of the following data sets:

(1) Volume mixing ratio vertical profiles for UV NO_2, UV O_3, Visible O_3;
(2) Aerosol extinction vertical profiles;
(3) Total optical depth spectra (UV and Visible);
(4) Aerosol optical depth spectra (Visible only);
(5) Water vapour volume mixing ratio vertical profiles;
(6) Angstrom coefficient vertical profiles.

This first release includes items (1) – (4).

2. Volume mixing ratio vertical profile data of UV NO_2, UV O_3, Visible O_3

As in v1.2 there are six volume mixing ratio vertical profile data products: NO_2 and O_3 from the UV spectrometer, O_3 from the Visible spectrometer. These data are provided at both the measurement and interpolated tangent heights.

The files can be obtained through the web-based download https://databace.scisat.ca/level2. One directory stores approximately one month of data. Note that a monthly directory may also contain data from the previous month. The date and time can be determined fully by the file name.

2.1 File naming convention

A file name is composed of the following information: orbit number, data type, date and time. For example, "ss2825_uno2_040220_172212_27.dat" reads: "SunSet Orbit ss2825, UV retrieved NO_2, measurement at 2004/02/20, 17:22:12UTC, using action table 27". (The action table number is likely irrelevant for general users.)

The data types can be identified in terms of sub-strings in the file names.

	Data type	
(1)	_uno2_	NO_2 profile retrieved from the UV spectrometer at the measurement tangent heights.
(2)	_uno2g_	NO_2 profile interpolated to a 0.5 km grid from the _uno2_ profile (1).
(3)	_uo3_	O_3 profile retrieved from the UV spectrometer at the measurement tangent heights.
(4)	_uo3g_	O_3 profile interpolated to a 0.5 km grid from the _uo3_ profile (3).
(5)	_vo3_	O_3 profile retrieved from the Visible spectrometer at the measurement tangent heights.
(6)	_vo3g_	O_3 profile interpolated to a 0.5 km grid from the _vo3_ profile (5).

The file names after Aug. 10, 2005 18:10UTC have an additional 'B' character before the two-digit action table number. This denotes the phase "B" measurement after that time when MAESTRO adopted a new measurement scheme (action table) of doubling the sampling rate for the significant altitude range. This should not be of relevance to general users.

For the SunRise data, the first two letters are "sr".

2.2 The data formats

The files are in ASCII columnar format. The data formats for products at measurement points and interpolated grids are slightly different:

1) At measurement points

Rows 11 and onwards are retrieved results with 6 columns in each entry.		
1	Index	Number of the data count.
2	Height	The MAESTRO measurement tangent height.
3	Nitrogen_Dioxide or Ozone	The retrieved Volume Mixing Ratio (VMR) in ppv (parts per volume). The values at 655 km, 100 km, and 0 km were obtained from the first guess. Bad data points are given by -1.#JE+000.
4	Error	The estimated fractional error transformed from instrument noise through the spectral fitting code and the vertical

		profile retrieval. This is estimated random noise and does not contain any systematic error component.
5	Ret	Flag for retrieved with 1, or not retrieved with 0. Values not retrieved are from the first guess profile.
6	Time	Elapsed seconds in the day.

2) At interpolation tangent heights

Rows 11 and onwards are interpolated results at finer grid with 5 columns in each entry.		
1	Index:	Number of the data count.
2	Height	Interpolated tangent height at finer grid from 0 km to 100 km.
3	Nitrogen_Dioxide or Ozone	Logarithmically interpolated Volume Mixing Ratio (VMR) in ppv from the measurement points.
4	Error	Fractional error interpolated from the tangent altitude values.
5	Retrieved?	Flag for retrieved with 1, or not retrieved with 0. Values not retrieved are from the first guess profile.

3. Aerosol extinction vertical profiles

Two aerosol extinction vertical profile data products were generated in version 3.12. They were derived from the Visible spectrometer at measurement tangent heights and then interpolated onto the 0.5 km altitude grid.

The files can be obtained through the web-based download https://databace.scisat.ca/level2. One directory stores approximately one month of data. Note that a monthly directory may also contain data from the previous month. The date and time can be determined fully by the file name.

3.1 File naming convention

A file name is composed of following information: orbit number, data type, date and time. For example, "ss2825_aepv_040220_172212_27.dat" reads: "SunSet Orbit ss2825, aerosol extinction vertical profile from Visible spectrometer, measurement at 2004/02/20, 17:22:12UTC, using action table 27". (The action table number is likely irrelevant for general users.)

The data types can be identified in terms of the fixed sub-strings in the file names.

(1)	_aepv_	Aerosol extinction vertical profiles derived from the Visible spectrometer at the measurement tangent heights.
(2)	_aepgv_	Aerosol extinction vertical profiles interpolated to a 0.5 km altitude grid from the _aepv_ profile (1).

The file names after Aug. 10, 2005 18:10UTC have an additional 'B' character before the two-digit action table number. This denotes the phase "B" measurement after that time when MAESTRO adopted a new measurement scheme (action table) by doubling the sampling rate for the significant altitude range. This should not be of relevance for general users.

For the SunRise data, the first two letters are "sr".

3.2 The data formats

The files are in ASCII columnar format. The data formats for products at measurement points and interpolated grids are slightly different. Aerosol extinction is provided in both direct extinction values (km^{-1}) and as extinction per unit air density ($km^{-1}molecules^{-1}cm^{3}$). In the latter unit the extinction ratio is approximately constant as a function of altitude for background aerosol.

1) At measurement points

Rows 13 and onwards are retrieved results with 26 columns in each entry.		
1	Index	Number of the data count.
2	Height	The MAESTRO measurement tangent height.
3 – 12	Aerosol extinctions at 10 selected wavelengths	The retrieved aerosol extinction (km^{-1}) vertical profiles at 10 selected wavelengths: 525nm, 530nm, 560nm, 603nm, 675nm, 779nm, 875nm, 922nm, 995nm, 1012nm. The values at 655km, 100km, and 0km were obtained from the first guess.
13	Retrieved	Flag for a successful retrieval at all wavelengths. Retrieved with 1, or not retrieved with 0.
14	Time_(s)	Elapsed seconds in the day.
15	Air Density	Number density of air (cm^{-3})
16-25	Aerosol in "mixing ratio format" for ten wavelengths	The retrieved aerosol extinction per unit air density ($km^{-1}molecules^{-1}cm^{3}$) vertical profiles at 10 selected wavelengths: 525nm, 530nm, 560nm, 603nm, 675nm, 779nm, 875nm, 922nm, 995nm, 1012nm. The values at 655km, 100km, and 0km were obtained from the first guess.
26	Flag	A combined flag for describing the 10 flags of the retrieved aerosol extinctions at the 10 selected wavelengths. Its value is Σ flag(n)$\cdot 2^{n}$, (n=0,…,9), flag(n) either 1 for "retrieved" or 0 for "not retrieved" for the n-th wavelength.

2) At interpolated regular grid

Rows 13 and onwards are retrieved results with 25 columns in each entry.		
1	Index	Number of the data count.
2	Height	The interpolated tangent height.
3 - 12	Aerosol extinctions at 10 wavelengths	The aerosol extinction (km^{-1}) vertical profiles at interpolated tangent heights at 10 selected wavelengths: 525nm, 530nm, 560nm, 603nm, 675nm, 779nm, 875nm, 922nm, 995nm, 1012nm.
13	Retrieved?	Flag for retrieved with 1, or not retrieved with 0.
14	Air Density	Number density of air (cm^{-3})
15-24	Aerosol in "mixing ratio format" for ten wavelengths	The retrieved aerosol extinction per unit air density ($km^{-1}molecules^{-1}cm^{3}$) vertical profiles at 10 selected wavelengths: 525nm, 530nm, 560nm, 603nm, 675nm, 779nm, 875nm, 922nm, 995nm, 1012nm.
25	Flag	A combined flag for describing the 10 flags of the retrieved aerosol extinctions at the 10 selected wavelengths. Its value is Σ flag(n)$\cdot 2^{n}$, (n=0,…,9), flag(n) either 1 for "retrieved" or 0 for "not retrieved" for the n-th wavelength.

4. The total optical depth data

The total optical depth data can be obtained through the web-based download https://databace.scisat.ca/level2. As for the mixing ratio data, the complete date and time information is fully coded in the file name.

4.1 File naming convention

The optical depth data have two files for each measurement. One is for UV, the other for Visible. The naming convention is similar to the volume mixing ratio files. For example, "ss2825_odu_040220_172212_27.dat" reads: "SunSet Orbit ss2825, Optical Depth for UV, measurement at 2004/02/20 17:22:12UTC, using action table 27". (The action table number is likely irrelevant for general users.)

For the corresponding Visible optical depth data, the sub-string "_odu_" is replaced by "_odv_".

The file names after Aug. 10, 2005 18:10UTC have an additional 'B' character before the two-digit action table number. This denotes the phase "B" measurement after that time when MAESTRO adopted a new measurement scheme (action table) by doubling the sampling rate for the significant altitude range. This should not be of relevance to general users.

For the SunRise data, the first two letters are "sr".

4.2 The data format

The files are in ASCII columnar format. Both UV and Visible optical depth data have the same format. The structure is as follows:

1	Rows 1-2	Two header lines of the file.
2	Row 3	One header line for one spectrum measurement. In this line, three parameters after "TIME:" are important. They are MAESTRO recorded date (yymmdd), time in UTC (hhmmss.). The third parameter is the corrected elapsed seconds of the day by incorporating the calculated MAESTRO/FTS time difference for this occultation.
3	Row 4	The tangent height in km at the time given in Row 3. Any missing altitude is filled with a default value of 999.9.
4	Rows 5 - 1022	The 1018 lines represent 1018 pixels of the optical depth. Each row is given by two columns: the first is the estimated wavelength in nm, the second the optical depth (unitless). The data gaps are filled with either the infinite number "1.#INF0e+000" or a Non-A-Number of "-1.#IND0e+000".
5	Repeat 2 - 4 for N times until end of file.	

5. The aerosol optical depth data

The aerosol optical depth data can be obtained through the web-based download https://databace.scisat.ca/level2. The date and time can be determined fully by the file name.

5.1 The file naming convention

The aerosol optical depth data have one file for each measurement – from Visible spectrometer only. The naming convention is similar to the volume mixing ratio files. For example, "ss2825_aev_040220_172212_27.dat" reads: "SunSet Orbit ss2825, Aerosol Optical Depth for Visible, measurement at 2004/02/20 17:22:12UTC, using action table 27". (The action table number is likely irrelevant for general users.)

The file names after Aug. 10, 2005 18:10UTC have an additional 'B' character before the two-digit action table number. This denotes the phase "B" measurement after that time when MAESTRO adopted a new measurement scheme (action table) by doubling the sampling rate for the significant altitude range. This should not be of relevance for general users.

For the SunRise data, the first two letters are "sr".

5.2 The data format

The Visible aerosol optical depth data have the following formats:

1	Row 1	One header line for one spectrum measurement. In this line, three parameters after "TIME:" are important. They are MAESTRO recorded date (yymmdd), time in UTC (hhmmss.). The third parameter is the corrected elapsed seconds of the day by incorporating the calculated MAESTRO/FTS time difference for this occultation.
2	Row 2	The tangent height in km at the time given in Row 3. Any missing altitude is filled with a default value of 999.9.
3	Rows 3 - 1026	The 1024 lines represent 1024 pixels of the optical depth. Each row is given by 4 columns: the first is the estimated wavelength in nm; the second gaseous optical depth spectrum; the third observed optical depth spectrum; and the 4th column the aerosol optical depth spectrum. The data gaps are filled with either infinite number of "1.#INF0e+000" or a Non-A-Number of "-1.#IND0e+000".
4	Repeat 1 – 3 for N times until end of file.	

6. Ancillary data

Ancillary data are those additional data associated with the measurement such as geolocation data. The linkage of the profile data or optical depth data with the ancillary data is through the common orbit number. The orbit number is the common key for linking all different types of data in ACE database.

6.1 Geolocation data

Two files "SunriseTable.txt" and "SunsetTable.txt" are lookup tables of partial geolocation information for each occultation in ASCII format. Each file contains six columns. They are:
-Orbit number
-Date
-Time in UTC at 30km tangent height
-latitude at 30km tangent height
-longitude at 30km tangent height
-beta angle

7. Previous versions

A version change is caused by these factors: 1) major forward model and/or retrieval algorithm changes; 2) Input data changes such as version changes of the input ACE-FTS retrieved pressure and temperature (p,T) profile data; 3) Changes of the tuning instrument parameters. Previous three data products released are:

Version 1.0: The first MAESTRO data product covers the period from Feb 2004 to May 2005. This version utilized various versions of ACE-FTS retrieved p,T profiles, e.g. versions 1, 2.0, 2.1, 2.2.

Version 1.1: This data set was produced uniformly based on version 2.2 of FTS p,T profiles and covers the period from Feb 2004 to Feb 2006. In the future this version will no longer be processed. Users are encouraged to use version 1.2 instead.

Version 1.2: This data product was based on FTS v2.2 p,T data for period from Feb. 2004 to Aug. 2011 and on FTS v3.0 p,T data from Sept. 2011 to Jul. 2012. Comparing to version 1.1 it utilized an optimal set of instrument parameters in time shift, UV spectrometer angle shift and VISIBLE spectrometer angle shift. The three shifts are relative to the ACE-FTS instrument. Nitrogen dioxide (NO_2) and ozone (O_3) mixing ratios as well as UV and VISIBLE optical depth are the routine products.

8. Reference

[1] McElroy C.T., C.R. Nowlan, J.R. Drummond, D.V. Barton, MAESTRO: The SCISAT UV-Visible-Near IR instrument, submitted manuscript, 2013.

[2] McElroy, C.T., C.R. Nowlan, J.R. Drummond, P.F. Bernath, D.V. Barton, D.G. Dufour, C. Midwinter, R.B. Hall, A. Ogyu, A. Ullberg, D.I. Wardle, J. Kar, J.Zou, F. Nichitiu, C.D. Boone, K.A Walker, N. Rowlands, The ACE-MAESTRO instrument on SCISAT: description, performance and preliminary result, Applied Optics, Vol. 46, No. 20, 2007.

[3] Kar, J., C.T. McElroy, J.R. Drummond, J. Zou, F. Nichitiu, K.A. Walker, C.E. Randall, C.R. Nowlan, D.G. Dufour, C.D. Boone, P.F. Bernath, C.R. Trepte, L.W. Thomason, and C. McLinden, Initial comparison of ozone and NO_2 profiles from ACE-MAESTRO with balloon and satellite data, J. Geophys. Res., **112**, D16, 1984–2012, doi: 10.1029/2006JD008242, 2007.

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