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**Earth Observing System (EOS)
Aura Spacecraft**

**TROPOSPHERIC
EMISSION SPECTROMETER
(TES)**

**Level 3 Algorithms,
Requirements & Products**

Version 2.0

April 20, 2005



**Jet Propulsion Laboratory
California Institute of Technology
Pasadena, CA 91109**

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**Level 3 Algorithms, Requirements
& Products**

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1. INTRODUCTION

1.1 Purpose of This Document

This document defines the TES (Tropospheric Emission Spectrometer) Level 3 data products and to describe the algorithms to generate the Level 3 data and the associated browsing images.

1.2 Related Documents

Tropospheric Emission Spectrometer: Science Objectives & Approach, Goals & Requirements. JPL D-11294, Version 6.0, April 1999.

Tropospheric Emission Spectrometer: Level 2 Algorithm Theoretical Bases Document. JPL D-16474, Version 1.1, October 1999.

Tropospheric Emission Spectrometer: Visualization Software Requirements. JPL D-xxxxx, Version 1.0, March 2001.

1.3 The TES Experiment on EOS Aura Satellite

The Tropospheric Emission Spectrometer (TES) is one of four instruments on board NASA EOS (Earth Observing System) Aura satellite scheduled for launch in early 2004. The other three instruments are the High Resolution Dynamic Limb Sounder (HIRDLS), the Microwave Limb Sounder (MLS), and the Ozone Monitoring Instrument (OMI). The objective of the EOS Aura Mission is to study the chemistry and dynamics of the Earth's atmosphere from the ground through the mesosphere (<http://aura.gsfc.nasa.gov>). The expected lifetime for the satellite is five years or longer.

TES experiment will provide long-term, vertically resolved global measurements of tropospheric ozone and its key precursors (Beer *et al.*, 2001). In the global survey mode, TES standard products include profiles of temperature, ozone, water vapor, CO, and CH₄ in the troposphere and stratosphere, NO₂, and HNO₃ in the mid-upper troposphere and stratosphere, the surface temperature and the spectral dependent surface emissivity in the infrared region. The global measurements of these profiles are essential in studying tropospheric ozone chemistry and the issues related to climate change, air pollution and greenhouse effects. TES data are of very valuable to the atmospheric research and other research and educational communities.

TES is an infrared, high spectral resolution Fourier Transform Spectrometer (FTS). It operates in both nadir and limb modes. Many detailed descriptions of the instrument and the measurements can be found in the documents listed in 1.2. In this document, only Level 3 related issues are discussed. To help processing developers and data users to

understand TES observations and its Level 2 and Level 3 data, the following Tables and Figures are provided to explain and illustrate the characteristics of TES observations and its coverages.

(1) The Aura orbit and the TES global survey strategy

The Aura orbit is sun-synchronous at 705 km altitude with a 98° inclination and 1:45 pm ascending equator-crossing time. Figure 1-1 illustrates TES observation location coverage for 16 orbits. The TES global survey operation will be a “one-day-on” followed by “one-day-off” pattern. Since there are about 14.5 orbits in a 24-hour period, the “on” period that actually lasts 16 orbits is about 26.5 hours. The global measurements of the atmospheric species will be provided every other day.

(2) Nadir and limb observations in a sequence

During each orbit, TES will make 72 “sequence” operations covering 82°S to 82°N latitude. Each sequence includes 2 calibration scans, and 2 nadir scans followed by 3 limb scans. Here “scan” refers to the mirror scanning performed inside the FTS instrument. TES will not do spatial scans for the purpose of covering more horizontal / altitude ranges. In the nadir case, the 2 scans point to a same ground location with the size of 8 × 5 km combining all detecting pixels. In the limb case, the 16 stacked detecting pixel detectors cover vertical range of about 35 km at the tangent with each pixel covering about 2.3 km, and the horizontal width is about 23 km at the tangent. The limb observations are pointed along the trailing view of the satellite.

Figure 1-1 illustrates the footprints for the nadir observations and the tangent locations for the limb observations. Associated with those locations, Table 1-1 summarizes the potential Level 2 profile data products. The two nadir observations are averaged to produce a single nadir product and the three limb observations in the sequence are analyzed separately. More discussions will be given in the next section (1.4).

Table 1-1. TES Level 2 Standard Products

Product	Nadir	Limb-1	Limb-2	Limb-3
Atmospheric Temperature, T	√	√	√	√
Surface Temperature, T _s	√			
Land Surface Emissivity	√			
Ozone (O ₃) VMR	√		√	√
Water Vapor (H ₂ O) VMR	√	√		
Carbon Monoxide (CO) VMR	√	√	√	√
Methane (CH ₄) VMR	√	√		
Nitrogen Dioxide (NO ₂) VMR			√	√
Nitric Acid (HNO ₃) VMR		√		

VMR — Volume Mixing Ratio

(3) Spatial resolutions for TES daily measurement

Aura orbit will repeat exactly every 16 days. The observation targets therefore repeat every 16 days. The orbit tracks are shifted in a 24-hour period. With the “one-day-on” followed by “one-day-off” strategy, a better “repeat coverage” is achieved. In other words, for a given target location on the 1st day, TES will come back to a closer location on the 3rd day compared to the 2nd day on which the measurement will be at a location that is between the two locations on the 1st day. On this “2nd day”, TES will be switched off for the purpose of extending its overall lifetime.

Figure 1-2 shows the latitude spacings of TES nadir footprints for an orbit. Between 60°S and 60°N, the latitude spacing is about 5°. The longitude spacing is illustrated in Figure 1-1. For a daily nadir observation, the longitude spacing varies between ~12° and ~24°. As it is stated above, the 3rd day’s coverage will not fill the gaps between the orbit track of the 1st day (Figure 1-1) and it will closely overlap with that of the 1st day.

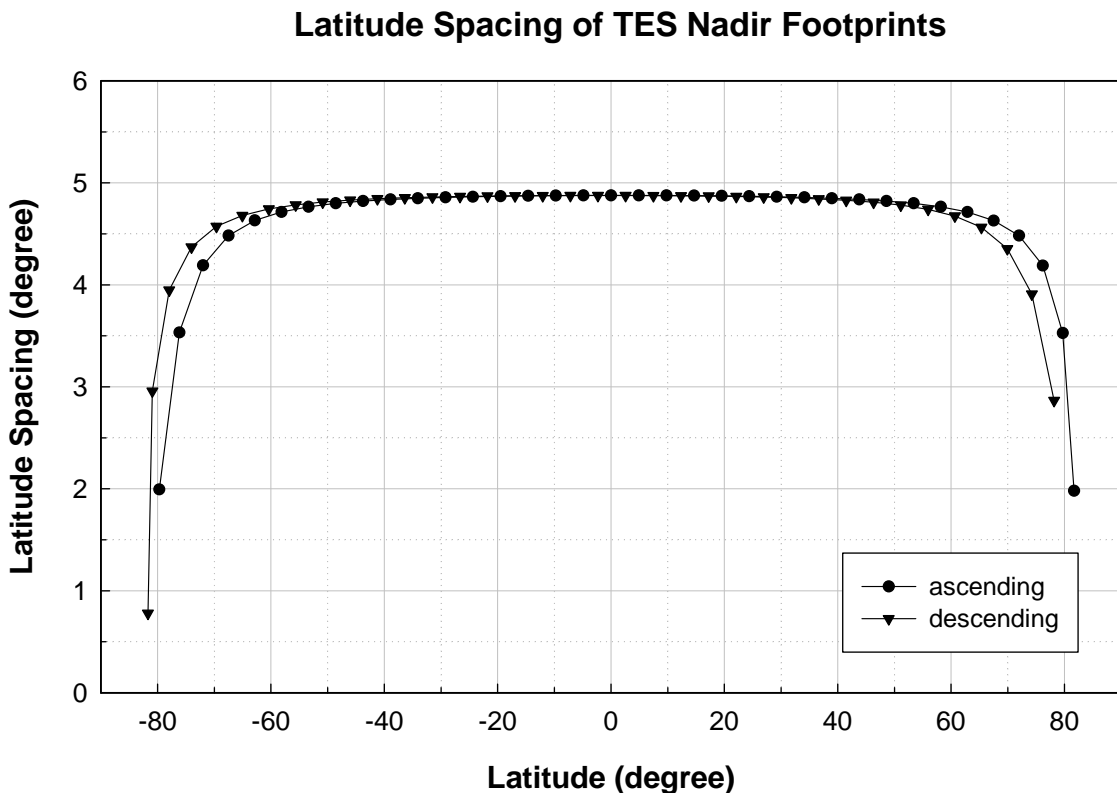


Figure 1-2. Latitude spacings of TES nadir footprints.

(4) Local times for TES global survey observations

The local solar times for a single orbit of TES observations are shown as a function of latitude in Figure 1-3. They are fixed throughout the mission. However, the local solar zenith angle at a given latitude varies following an annual cycle.

Most of the ascending (northward) observations are taken in the afternoon, within 3 hours after the noontime between 60°S and 60°N. Most of the descending (southward) observations are taken after the midnight, within 3 hours after 1:00 am between 60°S and 60°N.

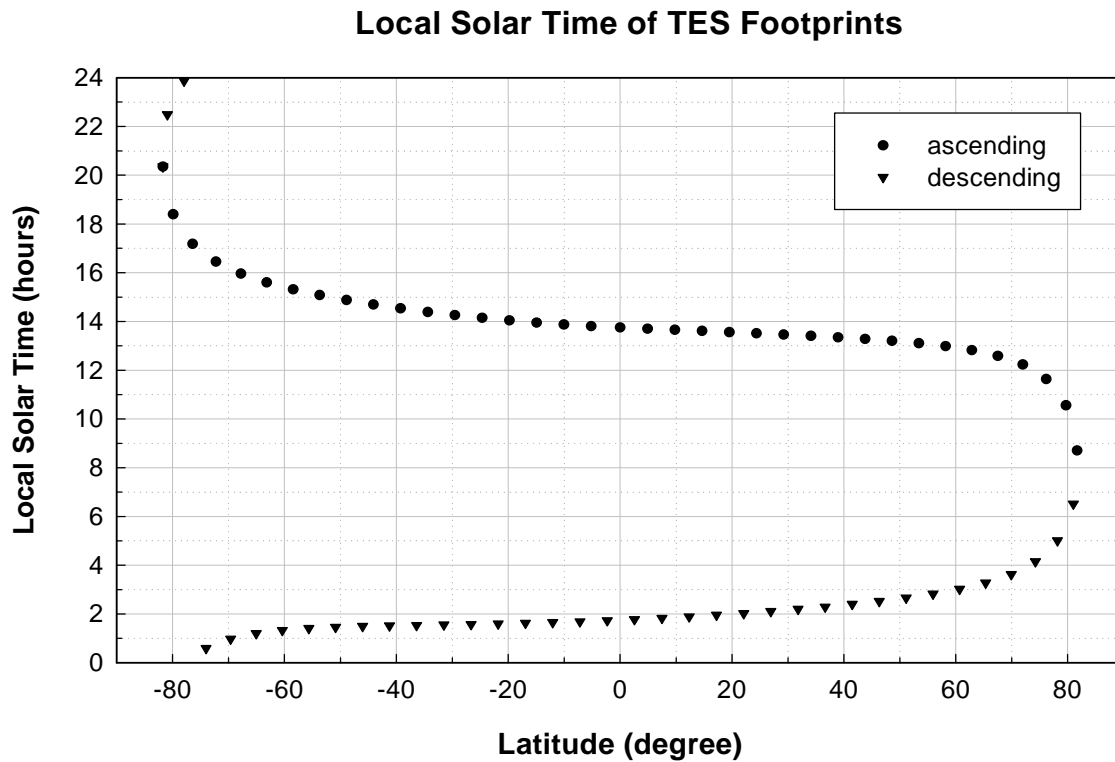


Figure 1-3. Local solar time as a function of latitude for a single orbit.

1.4 TES Data Products

TES distributed data have following stages.

- (1) Level 1B data are radiometrically calibrated spectral radiances corresponding to nadir or limb observation “scans” described above. The Level 1B processing is to

convert spectral radiances from measured interferograms including radiometrical calibrations.

- (2) Level 2 data are the retrieved atmospheric species profiles at the nadir footprint or the limb tangent. The Level 2 processing is to retrieve atmospheric temperature and species profiles via iteratively fitting an atmospheric radiative transfer model results with the observed spectral radiances (Level 1B data) considering the measurement noise and some known characteristics of the atmospheric parameters.

The Level 2 data are the inputs to Level 3 processing. Table 1-1 lists TES Level 2 global survey data products. The Volume Mixing Ratio (VMR) for chemical species is reported with respect to dry air. The vertical pressure levels of Level 2 data are UARS standard levels, defined as $P = 1000.0 \times 10^{-\frac{k}{6.0}}$ (hPa), where constant $k = 0, 1, 2, \dots$

The data granule for Level 2 data is a “daily” (actually 16 orbits) file per species. It includes time dependent data, such as the geolocations, solar zenith angles, and total column data *etc.*, and the time-pressure dependent profile data. The retrieval errors are also provided for the profiles.

- (3) Level 3 data are the “daily”, “8-day”, and “monthly” species profile (or the surface parameter and total column *etc.*) data interpolated into uniform longitude-latitude grid. A common grid of **4° longitude by 2° latitude** for Level 3 data is applied for all four instruments on the Aura spacecraft.

Per-GS, 8-day, and monthly image maps will be generated using Level 3 data. This document describes the algorithms, products, and requirements for the Level 3 processing.

1.5 TES Global Survey Strategy

TES global survey measurements are the TES routine measurements conducted every other day. This one-day “on” / one-day “off” pattern is determined by the requirement of five-year lifetime and the estimated 50% duty cycle based on the limitation of the total number of mechanical scans that the instrument can perform. A study of auto-correlations of the ozone and CO fields from a global three-dimensional tropospheric chemistry model and the global mappings for simulated TES samplings supports this decision (Luo *et al*, 2001).

More correctly, in an “on” period, the global survey measurements are performed 16 orbits contiguously. The time duration is about 26.5 hours. Figure 1-1 illustrates the geolocations of nadir and limb observations in this period. Ideally, there will be a Level 2 profile associated with each of these footprints. However, the measured spectra with cloud in the view will certainly create difficulty in the Level 2 retrieval processing. In the early stage of data production, these data will be flagged out for nadir case. Together

with missing data due to other reasons, there will be a lot of holes in the daily global coverage. Figure 1-4 shows two examples of coverages comparing an ideal daily nadir coverage and a simulated coverage with cloudy scene removed. The ozone data at 500 hPa is sampled from the GEOS-CHEM model developed at Harvard University (Bey *et al.*, 2001).

TES Level 3 data and global species image maps are generated for each “on” period of 16 orbits global survey. As described below, 8-day and monthly averaged Level 3 data and image maps are also generated.

1.6 Guidelines for Level 3 Product: Data and the Graphical Presentation

TES generated data at all three processing levels described briefly in 1.4 have various applications. The most important application for TES Level 3 data is to allow TES data users to be able to visualize global distributions of atmospheric species fields. The following guidelines are therefore presented here to guide the selections of Level 3 algorithm and products.

- (1) The main purpose of producing Level 3 gridded data is to generate daily, 8-day and monthly global maps of atmospheric parameters (*e. g.*, ozone VMR at a given pressure level, or the total CO column amounts etc.) for browsing or quick looks of the TES observation results.
- (2) Level 3 algorithms should preserve the field local variabilities in the troposphere captured in the collections of daily Level 2 data. The algorithms should be able to handle missing data in the “on” period (as high as 60% in the lower troposphere) and allow for non-data from “off” days.
- (3) The graphical representation of the Level 3 data is an important part of the TES Level 3 product. These global image maps (*e.g.*, .png files) will be distributed together with Level 3 data.
- (4) The data assimilation process combining TES Level 2 data and an atmospheric dynamical and chemical model is considered as TES “Level 4” processing. Level 3 data are not to be influenced by an atmospheric model. The Level 4 data will be generated on limited basis associated with the research interests and the available resources.

2. DEFINITION OF TES LEVEL 3 DATA AND VISUALIZATION PRODUCTS

2.1 Level 3 Data and the Images Associated with the Data

TES Level 3 product has two parts, the data and the viewing images produced using selected data. The file format for the data part is HDF-EOS-5.0, and the file formats for the image maps are PNG.

It is important for the Level 3 data users to understand the processing algorithm and its limitations. Although compared to Level 2 data, regularly gridded three-dimensional Level 3 data are convenient to use, it might be misleading in some applications. Users are encouraged to examine the global maps of geophysical parameters at Level 2 geolocations described next in 2.2.1 and the Level 3 global maps for the same parameters provided as a part of Level 3 product. These image maps are considered to be the most useful products in Level 3. Users are encouraged to access Level 2 data with retrieval uncertainties and other information for serious researches, such as data validation, correlation and trend analyses.

TES Level 3 products include daily, 8-day, and monthly products. The global image maps will not be able to display all the data in a given file. For example, only global images for a given species field at a few selected pressure levels will be generated. To explore data at all pressure levels, an interactive EOS-HDF viewer is recommended (section 4.2).

2.2 Daily and (or) 8-Day Products

This section describes the TES daily and 8-day products, data and image maps. All related Level 3 products are defined in Tables in sections 2.2.3 – 2.2.6 below. Section 2.2.1 describes the Level 2 daily global data visualization products.

2.2.1 *Daily Level 2 Data Global Visualization and Diagnostic*

As the first step to explore TES daily global measurements, graphical presentations of daily Level 2 profile data at selected pressure levels will be generated. These pressure levels will be the same as those used for Level 3 maps defined in the next section. Figure 1-4 shows two simulated examples of such plots, one without missing data likely to be for the limb observations above the cloud levels and nadir data above the cloud top, and the other with missing data due to cloud in the view and other reasons.

The global views of the cloud top pressures for nadir and limb at TES footprints are of useful in evaluating the vertical extends of the observations.

To assist the evaluations of Level 2 retrieval results, graphical forms of some diagnostic parameters will also be generated. The candidates include global plots of retrieval percent error, the difference between the retrieval results and the initial guess, and the chi-squares *etc.*

2.2.2 The Need for 8-Day Products

Although the primary goal for TES Level 3 processing is to provide daily global views of its measured parameters, problems expected in Level 2 retrievals when clouds are in the view of the instrument and other problems related to the initial instrument operations and data processing could result in reduced Level 2 daily data and therefore big gaps in the daily global coverage. For the products having diurnal variations, *e.g.*, ozone near the stratopause, NO and NO₂, the separation of ascending (day) and descending (night) data will further reduce the number of daily data points globally. The total column amount for the retrieved species profiles is another parameter that requires caution. The Level 2 reported total column is calculated from the bottom retrieval level to the space. This bottom retrieval level will be at the surface in clear-sky case and at the cloud top in the cloudy case respectively. Although displaying mapped global column data from all Level 2 daily results ignoring the vertical locations of the bottom retrieval levels has some value, the 8-day global column map generated from selected profiles retrieved all the way to the surface is perhaps more meaningful if the daily data coverage is not adequate enough to generate a global map. This argument also applies to level values in the low-middle troposphere.

In the above situations, producing Level 3 8-day data and image maps are necessary. The 8-day products are suitable for data browsing. In the following sub-sections, the Level 3 daily and 8-day products are commonly defined.

The time period used to accumulate TES Level 2 data to generate Level 3 8-day products is three consecutive global surveys.

2.2.3 Daily/8-Day Level 3 Data and Maps of Species at Defined Pressures

Table 2-1 lists the data files (HDF-EOS) and graphical image files (PNG) for Level 3 daily or 8-day pressure-level products.

**Table 2-1. Level 3 Daily/8-Day Pressure-Level Data and Images
(Horizontal grid: 4° longitude × 2° latitude between 82°S and 82°N)**

Product Name	Unit	# of pressure Levels for Data	Pressure Range for Data (hPa)	# of selected Pressure Levels for Image Map	Pressure Levels for Image Map (hPa)
temperature_nadir	K	15 & surf	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
H ₂ O_nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
O ₃ _nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col

CO_nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
CH ₄ _nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
temperature_limb	K	15	surf – 4.6	8	681,464,316, 215, 147, 100,46.4,10
H ₂ O_limb	vmr	15	surf – 4.6	6	681, 464, 316, 215, 147, 100
O ₃ _limb	vmr	15	surf – 4.6	8	681,464,316, 215, 147, 100,46.4,10
CO_limb	vmr	15	surf – 4.6	8	681,464,316, 215, 147, 100,46.4,10
CH ₄ _limb	vmr	15	surf – 4.6	3	464, 100, 46.4
NO ₂ _day_limb	vmr	15	surf – 4.6	3	100, 46.4, 10
NO ₂ _night_limb	vmr	15	surf – 4.6	3	100, 46.4, 10
HNO ₃ _limb	vmr	15	surf – 4.6	3	100, 46.4, 10

vmr – volume mixing ratio
surf – surface pressure

Since nitrogen dioxide (NO₂) has strong diurnal variation due to photo-chemistry of atmospheric nitrogen species, its day (ascending) and night (descending) data will be processed and plotted separately. Because NO₂ is zero at daytime the data for NO₂ used to generate a daily map will be about half of those used for other species. 8-Day data and images in this case could be very useful.

The 15 pressure levels for the above Level 3 data are the same as those in Level 2 profiles, defined as $P = 1000.0 \times 10^{-\frac{k}{60}}$ (hPa), where constant $k = 0, 1, 2, \dots, 14$. For a specific profile, the bottom pressure is the surface pressure, not necessarily to be 1000 hPa. The surface pressure array and the data at the surface will be provided in the daily/8-day Level 3 files.

2.2.4 Daily/8-Day L3 Data and Maps of Species Total Columns

Level 2 total column data and profile data are used to generate Level 3 total column data and images. Table 2-2 lists the parameters for Level 3 column data and associated images. These data files and images will be generated initially. As the TES science team examines and validates the global distributions of the nadir and limb columns, combined nadir-limb total column data / images may be generated in the future.

Table 2-2. Level 3 Daily/8-Day Column Data and Images*
(Horizontal grid: 4° longitude × 2° latitude between 82°S and 82°N)

H ₂ O_nadir	O ₃ _nadir	CO_nadir	CH ₄ _nadir			
H ₂ O_limb	O ₃ _limb	CO_limb	CH ₄ _limb	NO ₂ _day_limb	NO ₂ _night_limb	HNO ₃ _limb

* unit for column: molecule/cm².

* see text for more details.

Two types of Level 3 column data and images will be generated for nadir and limb respectively:

- (1) All Level 2 column data are used to produce Level 3 column maps; and
- (2) Selected Level 2 profile data are used to produce Level 3 column maps — *e.g.*, above surface for nadir and above 464 hPa for limb.

2.2.5 Daily/8-Day L3 Data and Maps of Surface Parameters

The TES Level 3 standard product for surface parameters is temperature (unit K) at the Earth surface measured in the nadir mode. The cloud top temperature in Level 2 data will not be included in Level 3 products. Daily and 8-day data and image maps will be generated for the surface temperature obtained in nadir retrievals. Separation of day and night (or roughly ascending and descending) data for image plotting of surface temperature may be necessary.

TES retrieval processing will also generate other surface parameters, such as spectral dependent surface emissivity. As non-standard product, Level 3 data and images will be produced for surface emissivity and (or) surface reflectance at defined spectral point (range).

~~2.2.6 Daily/Weekly L3 Zonal Mean Data and Images~~ **No Zonal Mean Products will be generated for Daily / 8-Day. Ignore this section.**

Daily or weekly Level 3 zonal mean data is the zonal average of Level 2 daily (weekly) data at all the longitudes at a given latitude range. The associated global latitude vs. pressure images for the zonal means of the atmospheric species are to be generated. Table 2-3 lists the names for these products.

Table 2-3. Level 3 Daily/Weekly Zonal Mean Data and Images
(Horizontal grid: every 2° latitude between 82°S and 82°N)

Product Name	Unit	# of pressure Levels for Data	Pressure Range for Data (hPa)	Pressure Ranges for Zonal Image Map (hPa)
temperature_nadir	K	15	surf – 4.6	1000 – 100, 1000 – 4.6
H ₂ O_nadir	vmr	15	surf – 4.6	1000 – 100
O ₃ _nadir	vmr	15	surf – 4.6	1000 – 100, 1000 – 4.6
CO_nadir	vmr	15	surf – 4.6	1000 – 100
CH ₄ _nadir	vmr	15	surf – 4.6	1000 – 4.6
temperature_limb	K	15	surf – 4.6	1000 – 100, 1000 – 4.6
H ₂ O_limb	vmr	15	surf – 4.6	1000 – 100, 100 – 4.6
O ₃ _limb	vmr	15	surf – 4.6	1000 – 100, 1000 – 4.6
CO_limb	vmr	15	surf – 4.6	1000 – 100, 100 – 10
CH ₄ _limb	vmr	15	surf – 4.6	1000 – 4.6
NO ₂ _day_limb	vmr	15	surf – 4.6	50 – 4.6
NO ₂ _night_limb	vmr	15	surf – 4.6	50 – 4.6
HNO ₃ _limb	vmr	15	surf – 4.6	1000 – 4.6

vmr – volume mixing ratio
surf – surface pressure

2.3 Monthly Products

The Level 3 monthly averaged data will be generated directly using Level 2 data. Here “month” means a calendar month.

Note: Tables included in Monthly Products are the same as those for daily/weekly now as placeholders.

2.3.1 Monthly L3 Data and Maps of Species at Defined Pressures

Table 2-4 lists the product names for the Level 3 monthly data and images. Like Daily Level 3 maps at defined pressures, monthly Level 3 species maps at the same set of defined pressures will be generated.

Table 2-4. Level 3 Monthly Pressure-Level Data and Images
(Horizontal grid: 4° longitude × 2° latitude between 82°S and 82°N)

Product Name	Unit	# of pressure Levels for Data	Pressure Range for Data (hPa)	# of selected Pressure Levels for Image Map	Pressure Levels for Image Map (hPa)
temperature_nadir	K	15 & surf	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
H ₂ O_nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
O ₃ _nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
CO_nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
CH ₄ _nadir	vmr	15 & col	surf – 4.6	7	surf, 681, 464, 316, 215, 147, 100, & col
temperature_limb	K	15	surf – 4.6	6	681,464,316,100,46.4,10
H ₂ O_limb	vmr	15	surf – 4.6	4	681, 464, 316, 100
O ₃ _limb	vmr	15	surf – 4.6	6	681,464,316,100,46.4,10
CO_limb	vmr	15	surf – 4.6	4	681, 464, 316, 100
CH ₄ _limb	vmr	15	surf – 4.6	3	464, 100, 46.4
NO ₂ _day_limb	vmr	15	surf – 4.6	3	100, 46.4, 10
NO ₂ _night_limb	vmr	15	surf – 4.6	3	100, 46.4, 10
HNO ₃ _limb	vmr	15	surf – 4.6	3	100, 46.4, 10

vmr – volume mixing ratio
surf – surface pressure

2.3.2 Monthly L3 Data and Maps of Species Total Columns

Monthly averaged Level 3 data and image maps for total columns will be generated for the same parameters of the daily/8-day column product (2.2.4). Table 2-5 gives such a list.

Table 2-5. Level 3 Monthly Column Data and Images
(Horizontal grid: 4° longitude × 2° latitude between 82°S and 82°N)

H ₂ O_nadir	O ₃ _nadir	CO_nadir	CH ₄ _nadir			
H ₂ O_limb	O ₃ _limb	CO_limb	CH ₄ _limb	NO ₂ _day_limb	NO ₂ _night_limb	HNO ₃ _limb

* unit for column: molecule/cm².

Only the column product (2) discussed in 2.2.4 will be generated.

2.3.3 Monthly L3 Zonal Mean Data and Images

The monthly averaged zonal mean data are generated from the daily Level 2 data. Same as the names of the data and the images for daily zonal means listed in Table 2-3, Table 2-6 lists the names for monthly zonal mean data and the images of latitude vs. pressure.

**Table 2-6. Level 3 Monthly Zonal Mean Data and Images (82°S – 82°N)
(Horizontal grid: every 2° latitude between 82°S and 82°N)**

Product Name	Unit	# of pressure Levels for Data	Pressure Range for Data (hPa)	Pressure Ranges for Zonal Image Map (hPa)
temperature_nadir	K	15	surf – 4.6	surf – 100, surf – 4.6
H ₂ O_nadir	vmr	15	surf – 4.6	surf – 100
O ₃ _nadir	vmr	15	surf – 4.6	surf – 100, surf – 4.6
CO_nadir	vmr	15	surf – 4.6	surf – 100
CH ₄ _nadir	vmr	15	surf – 4.6	surf – 4.6
temperature_limb	K	15	surf – 4.6	surf – 100, surf – 4.6
H ₂ O_limb	vmr	15	surf – 4.6	surf – 100, 100 – 4.6
O ₃ _limb	vmr	15	surf – 4.6	surf – 100, surf – 4.6
CO_limb	vmr	15	surf – 4.6	surf – 100, 100 – 10
CH ₄ _limb	vmr	15	surf – 4.6	surf – 4.6
NO ₂ _day_limb	vmr	15	surf – 4.6	50 – 4.6
NO ₂ _night_limb	vmr	15	surf – 4.6	50 – 4.6
HNO ₃ _limb	vmr	15	surf – 4.6	1000 – 4.6

vmr – volume mixing ratio

surf – surface pressure

2.4 Other Level 3 Visualization Products

The visualization products defined here are image plots (PNG files) generated using Level 3 data defined above. No data will be generated for these image plots. The visualization products described in this section will have secondary priority over the global images defined in 2.2 and 2.3.

2.4.1 Zoomed Daily Species Images in Specified Regions / Seasons

To examine TES data in more detail in interested regions and seasons to tropospheric chemistry, zoomed daily species images in pre-defined regions / seasons will be generated as part of Level 3 products. Compared to global view defined in 2.2.3 – 2.2.5, these zoomed images enhance the color contrast for smaller scaled features in smaller regions. Table 2-7 lists the tentative zoomed image products.

Table 2-7. Level 3 Zoomed Images

Product Name	Latitude/Longitude Boundaries	Time Peiod	Pressure Levels (hPa)
CO_nadir_E_Asia	TBD	Jan 1 – March 30	surf, 681
O ₃ _nadir_S_Africa	TBD	July 1 – Sept 30	surf, 681
O ₃ _nadir_USA	TBD	June 1 – Sept 30	surf, 681

2.4.2 Animation of Global / Regional Species Fields

The time series of daily, 8-day, or monthly Level 3 maps of species fields defined in 2.2.3 – 2.2.6, 2.3 and 2.4.1 can be displayed and recorded in an animated fashion. These yearly or seasonally long animation movies are considered as Level 3 visualization products. Detailed product contents are TBD.

2.4.3 Time Trends

The time-height or time-latitude cross-section images of a given field or the plot of a variable as a function of time are very useful in atmospheric researches as well as in monitoring the time trend of a given parameter. These graphics can be generated directly from TES Level 2 product or the Level 3 data. Detailed definitions are TBD.

2.5 Estimation of Data Volumes and Image File Sizes

Similar to Level 2 daily (16-orbit) product files, the file granule for Level 3 daily data will also be a single file per species. The Level 3 pressure-dependent data are three-dimensional: 90 longitude grids with 4° spacing, 83 latitude grids with 2° spacing between 82°S and 82°N, and 15 pressure levels with 6 levels every decade pressure between 1000 and 4.6 hPa. For the nadir observations, the surface pressure and the retrieved atmospheric parameter (*e.g.* species VMR) at surface are included in the data file. The Level 3 two-dimensional data are the global distributions of the total species columns and the surface parameters, and the zonal mean products. These products have

dimensions of 90 longitudes by 83 latitudes and 83 latitudes by 15 pressure levels, respectively.

To evaluate the data quality and monitor the Level 3 processing, an extra data field needs to be generated to store information produced in the processing. This diagnostic data field will be in the data file so that there will be 2 data records associated with each data grid described above.

Table 2-8 presents the estimated sizes for the Level 3 data files. Detailed product names are listed in Tables 2-1, 2-2 and 2-3 and in section 2.2.5. All Level 3 data will be 4-byte floating numbers. The grand total data volume for a single day (26.5 hours) when the instrument is powered on continuously for the global survey observations is about 15 Megabytes.

Table 2-8. Estimate of Data Volume for Daily Level 3 Data Files

Product Group	# of Data Files	Data Dimension	Size per File	Total Size (Megabyte)
Pressure-Level Data (Table 2-1)	13	90×83×(15+2)	1.0 MB	13
Total Column Data (Table 2-2)	22	90×83	60 KB	1.32
Surface Data (Section 2.2.4)	> 1	90×83	60 KB	> 0.06
Zonal Mean Data (Table 2-3)	13	83×15	16 KB	0.13
Daily Total Data Volume				15 MB

Table 2-9 presents the estimated sizes for the Level 3 image map files and the Level 2 images described in section 2.2.1. Detailed descriptions of Level 3 maps are in Tables 2-1, 2-2 and 2-3, and in section 2.2.5. The image sizes for all the maps are assumed to be 300 × 200 pixels. The grand total size for a single day's image maps is about 40 Megabytes.

Table 2-9. Estimate of File Sizes for Daily Level 3/Level 2 Image Map Files*

Product Group	# of Data Files	PS File Size per Image File	JPEG* File Size per Image File	Total Size (Megabyte)
L3 Pressure-Level Images (Table 2-1)	54	250 KB	75 KB	18 MB
L3 Total Column Images (Table 2-2)	22	250 KB	75 KB	7.2 MB

L3 Surface Param. Images (Sec 2.2.4)	> 1	250 KB	75 KB	> 0.3 MB
L3 Zonal Mean Images (Table 2-3)	19	250 KB	75 KB	6 MB
L2 Pressure-Level Images (Sec 2.2.1)	54	90 KB	60 KB	8.1 MB
Daily Total Size				40 MB

* based on **300 × 200 pixel** for global image maps, **sizes for PNG are yet to be estimated.**

55 Megabytes is estimated as the total size for Level 3 data and image files per day when TES operates. Since the 8-day and monthly products are very similarly defined as those daily products, the total file size for the 8-day and monthly products approximately equals to that for a single day's.

3. ALGORITHMS FOR GENERATING LEVEL 3 DAILY, 8-DAY, AND MONTHLY DATA

This section describes the algorithms used to generate Level 3 data defined in section 2. Several categories of possible algorithms that have been used on other earth science satellite data processing are reviewed in 3.1. Based on the guidelines described in section 1.6, we chose the 2-dimensional piecewise linear interpolation (3.3) as the primary method for generating daily L3 data and the binning averaging (3.4) method for generating zonal mean, 8-day and monthly data. Demonstrations of the two processing are given. These examples show that the algorithm defined here can very well preserve the large/small scaled features observable by TES at Level 2 footprints but produce a much better visual effect.

The Level 3 spatial grid is defined commonly for all the instruments on the Aura platform. This grid is 2° latitude by 4° longitude between 82°S and 82°N latitudes. It reasonably over samples the TES observations spatially.

The time offset between the daily observations will be ignored in Level 3 processing. No temporal interpolation will be done. The time tag for the Level 3 daily data is therefore the starting date. For diurnal varying species, such as NO₂, the average and the extreme local times for day and night data will be given.

The algorithm steps are described below in 3.2 – 3.4, and a processing flowchart is given in 3.5.

3.1 Brief Review of the Possible Algorithms

Many methods have been applied in generating global gridded data from irregularly sampled satellite data in space and time. Among many usages, the major application of generating those Level 3 data is that a global image map can be produced showing spatial-temporal variabilities captured by the observations. The characteristics of the fields are somewhat quantitative and depend on the choices of the algorithms. Here we briefly review several categories of algorithms previously used in generating Level 3 data, and we argue for choosing algorithms for TES Level 3 products based on guidelines presented in section 1.6.

Here we consider the mappings only on a constant pressure level, or for the surface parameters and total columns. No vertical interpolation is involved.

(1) Binning Average ignoring time variation

This is the most commonly used method to provide a quick look of the data. Within the considered time period associated with the data, the temporal variation is ignored. For each Level 3 grid point, a bin box is defined, and the data within the box is averaged. Weighting can be applied to each observed data, for example, weighted inversely by

distance and error. Together with the average for each bin, the standard deviation can be calculated describing the spread of the data within the bin.

The size of the bin depends on the average spacing between data locations. The bin should be large enough so that enough data points can be included in the bin, but it should also be small enough so that the local detail in the observed field can be identified. Overlapping the bins is a good way of compromising the two needs.

The weighted binning average method is an obvious choice for generating monthly, 8-day, and zonal mean global fields. In these cases, the average fields and the associated variability statistics are the interests in browsing and examining the longer-term trends in the observations.

This method could also be suitable for TES Level3 daily product, but the number of data points within a defined bin can be either none or as few as a couple of points. In this situation of non-overlapping sparse distribution, nearest neighbor interpolation is perhaps a better choice.

(2) Spatial Interpolation (C^0/C^1 continue) or estimate (minimize residual) ignoring time variation

The two dimensional spatial interpolation is the most straightforward way to fill the data gaps spatially when there are no overlaps in observed data locations. As shown in Figure 1-4, the accumulated TES contiguous 16 orbit data (~26.5 hours) for a given species cover entire globe. No location overlaps for this daily observation, ideal for 2-D interpolation.

The interpolation functions used to represent the global field should pass through all the observed data points (C^0 continue). Some interpolation functions are constructed to keep the 1st derivatives continue at the observed points (C^1 continue).

The spatial interpolation methods are also grouped into global and local methods. The difference of the two groups lies in the use of the observed data points, either all the data points globally or only a small sample of the data points. The visualization of the tropospheric observations requires that the interpolated global gridded data retain the small and large spatial details illustrated by the TES Level 2 data. It is therefore important to only consider local interpolation in the Level 3 processing.

The piecewise linear interpolation (C^0 continue) is the simplest interpolation method. In the spherical case, the modified Delaunay triangles consisting three nearby points for all the non-data area are constructed and the linear 2-dimensional interpolation is applied (details in 3.3).

There are other C^0/C^1 continue interpolation methods, such as the thin-plate splines and the higher degree of polynomials. Compared to the linear method, these methods fit the local or global data to smooth parameter surfaces. However, depending on the

distributions of the observed data, they tend to overshoot in data-poor areas, and occasionally create negative values as the result of the interpolation. Figure 3-1 illustrates four “realistic” situations using the analogue 1-D interpolation algorithms. All measurement data comes from the simulated TES samples of the ozone field at four narrow latitude bands (Figure 1-4). The original ozone fields are from the GEOS-CHEM model at Harvard University. The comparisons of the three interpolation algorithms clearly show that the simple 2-dimensional piecewise linear interpolation does not have potential overshooting problem and is adequate in representing the observed field for data browsing purpose.

Another method of fitting data in a 2-D surface is to pre-define a function representing the field and use the measurement data to find the parameters in the function via minimizing the residuals between the function and the data. Examples of the functions are the spherical harmonic or some kind of Fourier expansion. These functions are more suitable to be defined on a global scale, which would smear out the local features. The missing data cause very irregular sampling pattern, so the implementation for this fitting is difficult.

(3) Kriging ignoring time variation

The Kriging method for spatial interpolation is based on random function model consisting the nearby measurement points and the points to be estimated (Isaaks and Srivastava, 1989). The estimated value at a defined location is the weighted linear combination of nearby measurement points. The weights are calculated using a covariance function (*e.g.*, exponential) describing the correlations between each pair of observed points. The parameters for the function (nugget, range and sill) are to be decided, and they have some effects to the results.

The Kriging method is unfamiliar to most data users in tropospheric chemistry. Users would have to follow lengthy mathematical derivations to understand the algorithms. Compared to local interpolations, the degree of smoothing of the Kriging estimates is more severe. For 8-day or monthly data, the correlations between the observation points at different locations taken at different times are not very meaningful. Based on these considerations, the Kriging method will not be considered for use for TES Level 3 data processing.

(4) The Fast Fourier Synoptic mapping (Salby, 1982)

The Fast Fourier Transform synoptic mapping theory has been applied to satellite observations in the stratosphere (*e.g.*, the MLS data on the Upper Atmospheric Research Satellite, Jiang, 2000). This theorem uniquely relates combined asynoptic data (for an integer number of days) to their space-time spectrum and it proves that this spectrum coincide with that of equivalent, twice-daily synoptic sampling. The inverted twice-daily synoptic maps will capture the resolvable stationary zonal waves.

This method has difficulty dealing with data gaps in time and space. The under sampled features or the very localized features in the observed field will likely be smeared out in the recovered synoptic field. TES will only provide data every other day and 50-60% missing data in the nadir case is expected due to complications in retrievals when cloud is in the view. We will not, at least initially, apply the fast Fourier synoptic mapping method to generate Level 3 data.

(5) Simple Kalman Filter

In a very general sense, the following equations (Rodgers, 2000) express the problem that we are trying to solve:

$$\begin{aligned}x_t &= M(x_{t-1}) + \zeta_t \\y_t &= F(x_t) + \varepsilon_t\end{aligned}$$

where x_t is the atmospheric state that needs to be retrieved from the measurement y_t at time t , M_t is a known model describing the evolution of the field that transforms x_{t-1} into x_t , and ζ_t is a process noise term. The second equation is the measurement model, relating the measurement y_t with its experimental error ε_t to the state x_t , by way of a known forward model F_t .

The simple Kalman filter assumes the linear relations for the above two equations:

$$\begin{aligned}x_t &= Mx_{t-1} + \zeta_t \\y_t &= Fx_t + \varepsilon_t\end{aligned}$$

and the filter operates sequentially in t . x_t in the 2nd equation is optimally estimated using the 1st equation to obtain the a priori estimate of the state x_{at} and the covariance S_{at} .

An example of applying this method is the Level 3B data for some instruments on the Upper Atmospheric Research Satellite (UARS) (Reber, 1990). The state x_t in that case is represented by the coefficients of the Fourier expansion of the measurement data along a given latitude circle. The estimate sequence is for consecutive orbital measurement at the given latitude. $M = 1$ is applied in this case.

Similar to the Fast Fourier synoptic mapping, this method has difficulty to deal with data gaps in space and time. The small, localized features in the Level 2 data field are tend to be truncated out in the final global map.

(6) Global data assimilation using atmospheric chemistry model (optimal estimate or Kalman filter)

All the methods described above do not involve or involve very little about the knowledge that we have about the physical and chemistry processes in the atmosphere. Global data assimilation is such a process that combines an atmospheric model and the

satellite data, *e.g.*, TES Level 2 data, to derive the evolving global field for the interested species. Different form of the Kalman filter is one of the principles used in data assimilation (Rodgers, 2000), where M_t in (5) relating state x_t from state x_{t-1} is the chemistry model.

The data assimilation is a research process with the goals of validating and improving the atmospheric models or the knowledge about the dynamical and chemical processes in the atmosphere using satellite measurements. Since this process provides data at places and times that no satellite measurements are available and the results are based on the best knowledge about the atmosphere, it can also be a good tool for validating some satellite data against correlative measurements via other observation methods. The global data assimilation generates global maps of interested species. However, the results are model dependent, and they can be heavily weighted by the model in places and times that no measurements are available. We define these global products as the Level 4 products. To distinguish, the goal for the TES Level 3 products is to view or browse the TES global measurements minimally influenced by the prior knowledge about the species of interests.

3.2 Level 2 Data and Along Orbit Interpolation

The along orbit interpolation is the first step in TES daily Level 3 data processing. This spatial interpolation is a step to fill a portion of missing data. At a given pressure level, an ideal daily footprint distribution for nadir observations is shown in Figure 1-4 (a). However, there will be some missing data due to problems occurred from instrument operations to data processings in Level 1 and Level 2. In particular, TES observations cannot see through clouds. There will be no retrieved Level 2 data below the cloud top level when the cloud is in the field of view of TES. Figure 1-4 (b) gives an example of TES nadir footprints with about 56% cloudy scene removed [from Figure 1-4 (a)]. Along orbit interpolation will fill some of the gaps spatially in the daily data.

The along orbit interpolation will be carried out for a missing profile only when the two immediate adjacent observations are available, and it will be done separately for limb and nadir. The two adjacent observations along an orbit are the closest observations in time so the interpolation is proper. The interpolation will be linear interpolation in along-orbit distance between the given footprint with missing Level 2 data and the two adjacent footprints with Level 2 data. Other higher order interpolations are not considered because the distributions of the missing data are unpredictable.

Figure 3-2 (b) and (c) illustrates a result of this processing, where (b) shows the nadir locations of TES observations in 16 orbits and (c) shows the locations after the along orbit interpolation. This interpolation added 101 locations to the original 561 targets, a 18% increase.

3.3 Level 3 2-D Piecewise Linear Interpolation

The standard surface linear interpolation will be used to generate Level 3 daily gridded data from the irregularly sampled Level 2 data together with the along-orbit interpolated data (Figure 3-2c). Daily Level 2 data (16-orbit in about 26.5 hours) at a given constant pressure level are collected, ascending and descending together or separately, for the spatial interpolation ignoring the temporal variation. The along-orbit interpolation is performed before proceeding the following spatial interpolation.

The method of triangulation is to fit a plane through three sample points that surround the point being estimated. This linear equation for the plane is

$$L3_Data = a \cdot L3_longitude + b \cdot L3_latitude + c,$$

where coefficients for the plane function, a , b and c , are determined by the three nearby Level 2 data and their coordinates by solving three simultaneous linear equations.

The estimated value at a given Level 3 grid depends on which three nearby samples used to define the plane. The Delaunay triangulation is commonly used and it has the nice property of producing triangles that are close to equilateral as possible.

The values can be estimated for the locations inside the boundaries of a given Delaunay triangle. Although in general it is not proper to do extrapolations, it becomes necessary for the Level 3 grid points near our defined latitude boundaries, 82°S and 82°N.

In cases where Level 2 data are not available in large areas, the interpolations are not to be performed. The criteria defining the situation are TBD.

The diagnostic field associated with the Level 3 daily data can be the error propagated from Level 2 retrievals through linear interpolation though users need to be aware of the meanings of this error associated with assumptions applied to generate Level 3 data in time and space.

Figure 3-2 offers an example of applying the algorithm described in this section. The Harvard GEOS-CHEM model ozone daily average field at 500 hPa (a) is sampled at TES nadir observation locations with cloud in the view removed (b). The along orbit interpolation is performed shown in (c). This interpolation added 18% data points in the 16 orbits. The Delaunay triangulations for the along-orbit interpolated data are shown in (d). The Level 3 global map generated using surface linear interpolation within Delaunay triangles is shown in (e). (f) shows the percent differences between the model field and the Level 3 field, and (g) presents the histogram for the percent differences. In about 28% area, the difference is less than 5%; in about 51% area, the difference is less than 10%; and in 78% area the difference is less than 20%. The Level 3 map (e) adequately fulfilled the requirement of viewing TES daily (16-orbit) measurements (b) in a global scale.

3.4 Level 3 Spatial Binning / Weighted Averaging

The method described below will be used to generate Level 3 zonal mean, the global 8-day mean data, and the global monthly mean data. Level 2 data, not daily-interpolated Level 3 data, will be used for deriving these average fields. All the averages are done on a given constant pressure level or at the surface and for the total column.

The binning / weighted averaging method is carried out in following way. For a given pressure level of a species field, Level 2 data for the considered time period are collected. We then define a bin box with pre-defined latitude and longitude widths (degree). This bin box is centered at each Level 3 grid. The Level 2 data within the range of the bin are used for averaging. Each of these Level 2 data in the bin is weighted by the inverse of the distance between the Level 2 data point and Level 3 grid point (d_i) and the inverse of the retrieval variance (σ_i^2). The retrieval variance used here is the diagonal elements of the estimated error covariance matrix associated with each profile retrieval. In case of no Level 2 data in the bin box there will be no Level 3 data at that grid point. Bellow is the formula that describes the method.

$$L3_Data = \sum_i^{N_{binBox}} w_d(1/d_i) w_e(1/\sigma_i^2) L2_Data_i ,$$

where N_{binBox} is the total number of Level 2 data in the bin box, and $w_d(1/d_i) w_e(1/\sigma_i^2)$ are the weighting functions for inverse distance and retrieval error respectively.

The latitude and the longitude widths for the bin box need to be decided. It is very likely that the adjacent bin boxes overlap to compromise the needs for having enough data points in a given box and to resolve possible details in the data. These parameters should be made adjustable for experiments on real data before Level 3 data are to be produced.

To represent the spread of the data within a given bin box, the standard deviation is calculated via the following equation,

$$\sigma_{L3_Data} = \sqrt{\frac{1}{N_{binBox}} \sum_i^{N_{binBox}} (L2_Data_i - L3_Data)^2} .$$

This standard deviation will be provided together with the averaged data (L3_Data). The error propagated from individual retrievals to the average is less meaningful than the above parameter so it will not be provided.

The Level 2 nadir and limb data will be processed separately. The main reason is due to their different vertical resolutions. It is also important to view the global distributions of a given geophysical parameter, *e.g.*, tropospheric ozone volume mixing ratio, obtained in nadir and limb for the same time period separately for validation purposes.

In the nadir case, the surface level is a special level. Same binning/averaging algorithm will be used to calculate the surface pressure at the Level 3 grid points and to calculate the Level 3 data values at the surface. These two fields will be included in the Level 3 data files.

The bin box for generating zonal mean data is just one-dimension. The distance can be considered as along the meridian great circle.

3.5 Summary and Data Processing Flowcharts

Figure 3-3 shows the flowchart for Level 3 data processing and image generation. All the processings are shown in oval-shaped boxes and all the Level 3 data and image maps are shown in rectangle-shaped boxes.

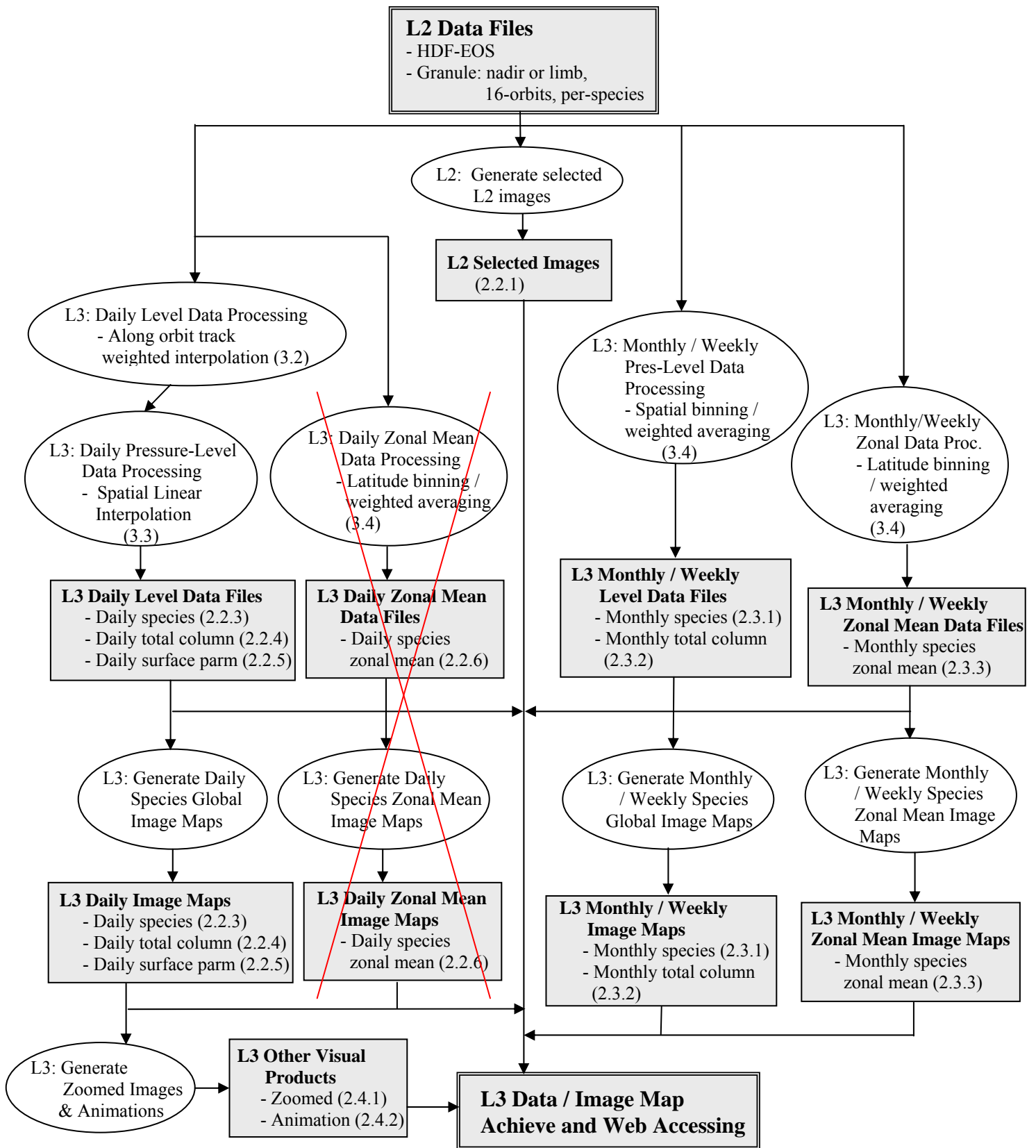


Figure 3-3. Flowchart for Level 3 data processing and image generation.

4. OTHER ISSUES

Within the TES observing system, Level 3 is perhaps the final step in delivering measurement results. The Level 3 processing algorithms applied for TES data will generate reasonable global distribution maps for the targeted species with limited spatial and time resolutions. Although Level 3 data will be made available, as data-browsing products, the Level 3 image maps are of more useful than the data set itself to both general public and researches who will examine TES data quantitatively. In this section we describe other issues and requirements that relate to Level 3 data/image validation and delivery.

4.1 Web Accessing of Level 3 Maps

The Level 3 image maps for TES observed species field defined in this document are the most commonly demanding graphical representations of TES data in the atmospheric chemistry community. Producing these image products and making them easily accessible to TES data users will greatly enhance the impact of TES observations to the tropospheric and other researches. This data browsing capability will save tremendous resources that many users would use to explore the data in a similar way.

Accessing the Level 3 image maps through the World Wide Web Internet is required. This involves the design of the accessing interface, data/image searching, and display mechanism. We will work with EOS DACC and EOS Data Gateway to implement the requirement.

4.2 Interactive Data Analysis and Visualization Tools

The Level 3 daily, 8-day and monthly data files are in HDF-EOS format. Many freely and commercially available products can be used to examine these data. TES team will identify one or two such a tool to examine Level 3 data.

4.3 Level 3 Data Validation

Level 3 data represent the global distributions of TES standard products listed in Table 1-1. The validation of Level 3 data involves two aspects. The first step is to compare the Level 3 data against Level 2 data. This can be done by visually comparing the plot of Level 2 species fields at their daily footprints (*e.g.*, Figure 3-2b) and the Level 3 global species images (*e.g.*, Figure 3-2e). The large-scale features in a Level 2 species field should be clearly captured in its Level 3 global image. The small-scale features represented by one or two footprints in the Level 2 field should also be captured in the Level 3 image.

The next step of validating Level 3 data is to compare with other sources of data in a global scale. This process should be based on the Level 2 data validation that is complicated by the differences in the vertical/horizontal resolutions, the timing, and the geolocation coincident of all sources of data involved. The comparison can be done in a qualitative sense or a more quantitative sense, and these two methods should be applied to different sources. In the qualitative sense, the two global image maps and their difference maps will be compared visually. In a more quantitative sense, the other data, *e.g.*, time varying 3-dimensional model data, can be re-sampled to TES footprints and observation times and then to form the global gridded data to compare with TES Level 3 data field.

Here is a list of potential data sources that could be used for validating Level 3 gridded global data.

- (1) Global daily, 8-day, and monthly Level 3 data from other instruments on the Aura platform, MLS, HRDLS, and OMI.
- (2) Global daily/monthly data from other satellite that overlaps with Aura in time, *e.g.*, Terra, Auqa, EnviSat, SAGE III, GIFTS, ...
- (3) Global climatology data from other satellite observations, *e.g.*, UARS ...
- (4) Global climatoloty / regional seasonal data from ground based / aircraft / balloon campaigns, *e.g.*, the ozone and CO climatologies from J. Logan ...
- (5) Assimilated data set using TES Level 2 results and other data.
- (6) 3-Dimensional tropospheric chemistry models.

4.4 TES Image Gallery

The TES image gallery should be created for general public and data users to better understand TES experiment and its capability. This gallery plays significant role in promoting and publicizing TES observations in its pre- and post- launch periods. The images and movies in the TES Image Gallery include art works explaining TES observations and the graphical representations of TES data easily understood by the general public. Most of the images in the TES Image Gallery are not TES Level 3 standard image products. A separate effort is therefore needed for generating images / movies for the TES Image Gallery.

The contents of TES Image Gallery will evolve with time. Selected Level 2 and Level 3 images are good candidates in the post-launch period. The graphical forms of field correlations and time trends are very valuable in examining and demonstrating TES data.

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