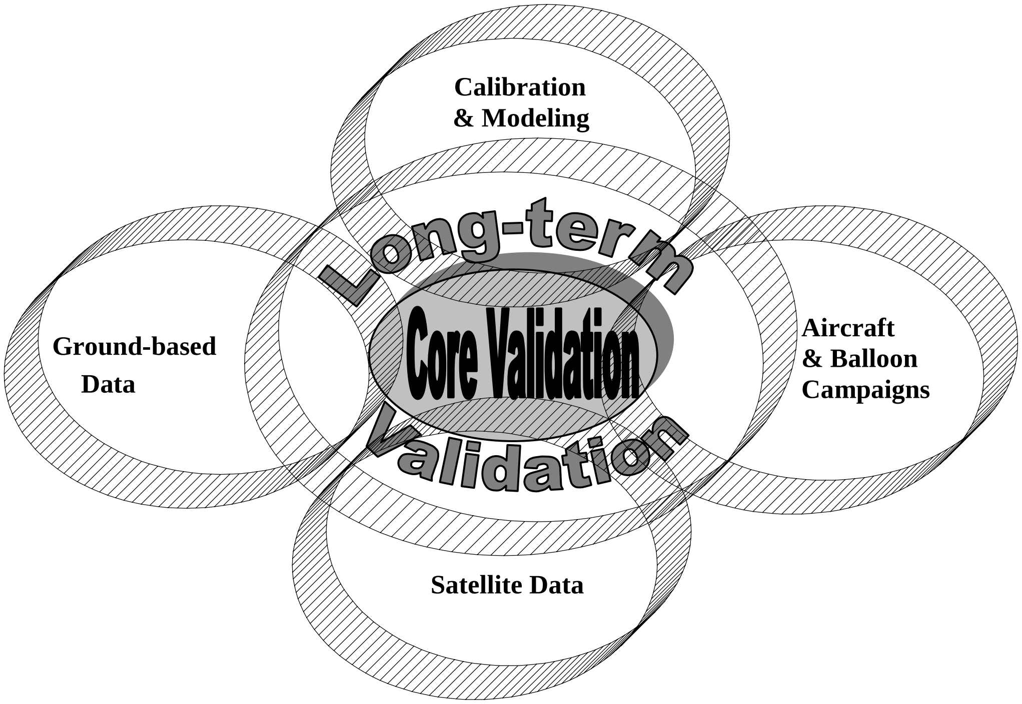
Earth Observing System (EOS)

Aura Science Data Validation Plan



Version 1.0
July 12, 2001

EOS Aura Science Data Validation Plan

Executive Summary

I. The Aura Mission

The Aura satellite is scheduled to be launched in 2003 in a sun-synchronous polar orbit for a nominal mission of five years. The four Aura instruments are: the High Resolution Dynamics Limb Sounder (HIRDLS), measuring infrared emission profiles from high resolution atmospheric limb scans behind Aura; the Microwave Limb Sounder (MLS), obtaining limb emission profiles ahead of the satellite; the Ozone Monitoring Instrument (OMI), a nadir-viewing UV/VIS imaging spectrometer with high spatial resolution; the Tropospheric Emission Spectrometer (TES), a Fourier Transform infrared spectrometer measuring in both the nadir and the limb mode behind Aura.

Section 2 of this document gives the Aura science goals, a description of the instruments and measurement characteristics. The top-level objectives are to resolve the following science questions:

- **Is the ozone layer changing as expected?**
- **Do we understand the transport of gases within the stratosphere and between the stratosphere and troposphere?**
- **What are the sources and distributions of tropospheric pollutants?**
- **What are the roles of upper tropospheric water vapor, aerosols, and ozone in climate change?**

The main products from Aura will be:
(1) Stratospheric profiles of temperature, O_3, H_2O, OH, HO_2, CH_4, CO, HCN, CH_3CN, N_2O, HNO_3, NO, NO_2, N_2O_5, HCl, ClO, $ClONO_2$, HOCl, CF_2Cl_2, $CFCl_3$, BrO, and aerosol extinction;
(2) Tropospheric profiles of temperature, O_3, H_2O, CH_4, CO, and HNO_3; upper tropospheric observations of NO, NO_2, and HCN; tropospheric column densities of O_3 and NO_2.
(3) Column densities of O_3, NO_2, HCHO, BrO, OClO.
(4) aerosol optical thickness.
(5) cloud information.
(6) volcanic SO_2.
Section 3 provides more details about these products and their expected uncertainties.

II. Summary of Aura Plans for Pre-launch Activities

Three major pre-launch activities that are necessary for successful (post-launch) validation of Aura products are: (1) Instrument calibration, (2) Algorithm testing, and (3) Compilation of spectroscopic data and other databases. These are discussed in section 4.

II.1 Instrument Calibration

Instrument calibration is closely tied to the continuing hardware development and testing of the Aura instruments. Each instrument will have detailed specific issues and schedules to follow. Pre-launch instrument and Project reviews and reports provide the means to assess the progress of the calibration plans that are briefly discussed (section 4.1).

II.2 Algorithm Testing

Pre-launch algorithm testing is discussed in section 4.2. The success of this testing directly impacts the quality of processed data after launch. Current test plans are summarized for each instrument team's algorithm. Where feasible, algorithms will be tested on data obtained by earlier satellite instruments. Algorithm mathematical approaches and some accuracy estimates are given in the Algorithm Theoretical Basis Documents. The Algorithm Working Group will guide some of the common activities (e.g., the use of a common model atmosphere for simulations and end-to-end testing), but much of the detailed work rests within each instrument team. Updates regarding algorithm status are ongoing and planned on a regular basis before the launch-ready software deliveries.

II.3 Spectroscopic Data and Other Databases

Databases of interest to the Aura instrument teams are identified, along with needs for new spectroscopic data (section 4.3). Since spectroscopic data generally come from outside the instrument teams, such needs were recently included as part of a NASA Research Announcement towards validation of data from the Aura and Aqua platforms. Through this and similar efforts, it is expected that many of the desired improvements in these databases will be met before the Aura launch. However, some important items (notably, information on the challenging HNO_3 infrared bands of relevance to both HIRDLS and TES, and on O_2-O_2 visible absorption cross sections for OMI) will require more attention in order for the satellite measurement accuracy requirements to be met. As each instrument team stays abreast of the uncertainties that remain in these databases, proper estimates of expected post-launch accuracy in the retrieved geophysical products can be made; this is a crucial and time consuming aspect of the validation assessments.

Other pre-launch activities currently underway include the gathering and/or development of data sets for use in the retrievals and/or simulations (climatology, operational meteorological data, or model values), coincidence predictor software, as well as gathering of other databases such as surface albedo and emissivity.

II.4 Models

Atmospheric models have several pre-launch applications to Aura validation. Constituent fields from atmospheric models will be used in synthetic data needed for algorithm testing. These constituent fields will also be used to develop strategies to obtain optimal information from comparisons of correlative observations with Aura measurements, especially in the upper troposphere and lower stratosphere where temporal and spatial scales of variability are much smaller than in the middle and upper stratosphere. Model fields will be used to develop quantitative requirements for coincidence criteria and also to develop statistical methods of comparison.

III. Summary of Aura Plans for Post-Launch Activities

The following paragraphs summarize the plans for validation activities following Aura launch as given in more detail in section 5. This plan will evolve and will include plans for correlative data location/extraction, formats, and data exchange protocols (section 6), as well as coincidence predictor software (also mentioned in section 4). Some of the specifics of this planning will have to await further definition of the investigations to be selected in support of Aura validation and science.

III.1 Aura Measurements and Validation Overview

Tables I.1, I.2, and I.3 summarize the measurements needed for validation of stratospheric profiles, tropospheric profiles, and column densities and other needs, respectively. Expected satellite, ground-based, and sonde data sources and opportunities are listed generically (for more details, see Table 5.3), with columns for satellite and ground-based data indicating expected amounts and quality/extent of match with Aura data. A priority column (with 1 for high, 2 for medium, 3 for lower priority) is used to indicate correlative data need as well as scientific importance of the Aura measurements (based on section 5.2.3.2). More details for each product can be found in section 5.2.3.3.

Although a significant number of tropospheric chemistry campaigns have occurred in the 1990's, there are no global data bases for most tropospheric constituents. Validation activities for tropospheric data are necessary over a broad range of latitudes and seasons.

III.2 Aerosols and Clouds

Besides the scientific interest in aerosols and clouds, these particles can affect the retrievals of other Aura products in the lower stratosphere and troposphere. OMI is sensitive to light-absorbing lower tropospheric particles (desert dust, particles from fires); HIRDLS and TES will sense stratospheric sulfate, polar stratospheric cloud, and upper tropospheric cirrus particles; the MLS experiment senses large particles (larger than 100 μm). A key validation source for the OMI experiment will be the aerosol optical thickness and single scattering albedo values measured by the AERONET set of ground based instruments. The primary measurements desired for HIRDLS and TES are particle size measurements of sulfate, PSCs, and upper tropospheric cirrus, and lidar measurements of aerosol spatial distributions, as well as other satellite observations of the extinction of the three types of particles. Correlative tropospheric aerosol composition information would also be useful. For the MLS cloud ice and OMI cloud products, the primary validation will use data from the Earth System Science Pathfinder (ESSP) Project mission CloudSat and ESSP3 (formerly PICASSO-CENA), but for MLS campaigns including cloud measurements of large ice particles are desirable. Measurements of the composition of stratospheric PSCs would allow us to relate satellite spectral information to composition.

III.3 Column Densities

The most important**,** currently unmet, validation need for OMI column densities is for tropospheric NO_2 under polluted as well as clean conditions; tropospheric ozone column densities are also desirable, as part of Aura-related campaigns. Under polluted NO_2 conditions, column and profile information in the lower troposphere is essential for the column density validation. Choices for this validation requirement are currently limited.

The ozone column measurement, also high priority, can be validated by Brewer Dobson instruments, integrating sonde measurements or by comparison to other satellite measurements (i.e. TOMS, GOME, SCIAMACHY). Again, not many of these instruments are located in very polluted areas, thus additional measurements are needed.

An aircraft campaign (e.g., with a UV-VIS DOAS-type instrument aboard) in which measurements of tropospheric and stratospheric profiles and column densities of NO_2 and O_3 are performed, can be used for these purposes (see also III.8 and III.9).

Table I.1. Aura stratospheric measurements and validation plans. Priorities (1, high; 2, medium; 3, lower) are for validation needs, with a consideration of scientific importance; a bracket indicates routine data are likely to provide significant/sufficient validation. *Correlative data sources and opportunities:* column **S** is for satellite data: ++ = sufficient/significant amount, + = moderate amount (some extra efforts may be needed), **-** = small amount or poorly matched (without extra efforts, proper validation cannot be performed); column **G** is for ground-based data, including sonde networks: "(C)" = column data with significant stratospheric contribution, "(c)" = column data of more marginal use for stratospheric validation. Column **B** (when filled in) represents a need/desire for balloon correlative data (X or D for existing capability or development needed); column **A** is for a similar need/desire for aircraft correlative data (lower stratosphere).

Parameter	**Priority**	**HIRDLS**	**MLS**	**TES**	**OMI**	**S**	**G**	**B**	**A**	**Comments**
Temperature	[1]	●	●	●		++	++	(X)	(X)	Sufficient correlative data (e.g., Op. Met., GPS, ARM data).
O_3	[1]	●	●	●	●	++	++	(X)	(X)	Campaign-derived horizontal gradients for profiles very desirable (lower strat.). Maintain existing ozonesonde programs.
H_2O	1	●	●	●		++	+	X	X	Campaign-derived horizontal gradients for profiles very desirable (lower strat.). Balloon profiles at range of latitudes are needed.
N_2O	1	●	●	●		++	-	X	X	Balloon profiles very desirable.
CH_4	1	●		●		++	-(c)	X	X	Balloon profiles very desirable.
HCl	1		●			-	-(C)	X	X	Balloon profiles very desirable.
OH	1		● (*)			-	-(C)	X	X	Balloon profiles very desirable.
HNO_3	1	●	● (*)	●		++	-	X	X	Balloon/aircraft data very desirable.
BrO	1		● (**)			+	-(C)	X	X	Balloon profiles very desirable.
Aerosols, PSCs	1 (see comment)	●		●		++	+	X	X	In part for spectral information and retrieval needs. High need for aerosol data if large volcano erupts.
ClO	2		● (*)			-	-	X	X	Balloon/aircraft profiles desirable (polar vortex also).
$ClONO_2$	2	●		● (1)		++	-(C)	X	X	Balloon/aircraft profiles desirable (polar vortex also).
CFC-11, CFC-12	2	●				++	-(c)	X	X	Balloon/aircraft profiles desirable.
HOCl	2		● (**)			-	-	X	X	Few correlative data. Balloon profiles desirable.
HO_2	2		● (**)			-	-	X	X	Few correlative data. Balloon profiles desirable.
NO	2			●		-	-(c)	X	X	Balloon profiles (non-twilight data) desirable.
NO_2	2	●		●		++	-(c)	X	X	Balloon profiles (non-twilight data) desirable.
N_2O_5	2	●				+	-	X	X	Few correlative data. Balloon profiles desirable.
CO	2		● (*)	●		++	-(c)	X	X	Some balloon profiles desirable (e.g., in polar vortex).
HCN	3		● (*)			-	-(c)	X	X	Few correlative data. Balloon profiles desirable.
CH_3CN	3		● (**)			-	-	X/D	X/D	Few correlative data.
SO_2 (volcanic)	3		● (*)			+	-	(X)	(X)	Only important if stratospheric volcanic plume is generated.
Geopotential Hgt	[3]	●	●			++	++			

(1) Not a standard product, at least initially (requires more time/research). (*) This measurement often requires averaging. (**) This measurement always requires averaging.

Table I.2. Aura tropospheric measurements (C_{trop} = tropospheric column density, with a validation need for profiles) and validation plans.
Priorities (1, high; 2, medium; 3, lower) are for validation needs, with a consideration of scientific importance; a bracket indicates routine data are likely to provide significant/sufficient validation. *Correlative data sources and opportunities:* column **S** is for satellite data: ++ = sufficient/significant amount, + = moderate amount (some extra efforts may be needed), - = small amount or poorly matched (without extra efforts, proper validation cannot be performed); column **G** is for ground-based data, including sonde networks. Column **B** (when filled in) represents a need/desire for balloon correlative data (X or D for existing capability or development needed); column **A** is for a similar need/desire for aircraft correlative data (troposphere). Other balloon/aircraft needs are listed for the lower stratosphere in Table I.1 (the Aura products below generally extend into the stratosphere).

Parameter	**Priority**	**HIRDLS**	**MLS**	**TES**	**OMI**	**S**	**G**	**B**	**A**	**Comments**
Temperature	[1]	● (2)	● (2)	●		++	++	X	X	Temperature data desirable in conjunction with other correlative tropospheric observations.
O_3	1	● (2)	● (2)	●	C_{trop} (1)	+	+	X	X	Campaign-derived horizontal gradients for profiles and tropospheric columns very desirable. Maintain existing ozonesonde programs.
H_2O	1	● (2)	● (2)	●		++	++	X	X	Campaign-derived horizontal gradients for profiles very desirable.
CO	1		● (2) (*)	●		+	+	X	X	Desirable to follow up on correlative data program similar to the one for MOPITT.
HNO_3	1			●		-	-	X	D	Few correlative data sources, none in lower troposphere; aircraft profiling very desirable.
NO	1			● (2)		+	-	X	X	Few correlative data. Diurnal effects are an issue.
NO_2	1			● (2)	C_{trop} (1)	+	-	X	X	Few correlative data. Diurnal effects are an issue. For OMI, tropospheric columns and profiles are needed for validating column densities in polluted regions.
Cloud properties	1	● (1)	● (1)	● (1)	●	+	-	X	X	In-situ data on cloud particle size distributions desirable. For OMI, the optical thickness of clouds, cloud albedo, & information about cloud system structure are desirable.
Cloud detection	[1]	●	●	● (1)	●	++	-			
Aerosols	1 (see comment)	● (2)		● (1)	●	+	+	X	X	Needed for aerosol product validation, but also for spectral information and other product retrieval needs. In-situ data on aerosol particle size distributions and composition desirable.
CH_4	2	● (2)		●		+	+	X	X	Desirable to follow up on correlative data program similar to the one for MOPITT.
HCN	2		● (2)			-	-	X	X	Few correlative data sources; profiles desirable.
N_2O	[2]	● (2)				-	++			Surface measurements adequate for troposphere.
CFC-11, CFC-12	[2]	● (2)				-	++			Surface measurements adequate for troposphere.
Geopotential Hgt	[3]	● (2)	● (2)			+	++			

(1) Not a standard product, at least initially (requires more time/research). (2) No measurement below the upper troposphere. (*) This measurement often requires averaging.

Table I.3. Aura column density and other measurements (C = column density, C_{trop} = tropospheric column density) and validation plans. Priorities (1, high; 2, medium; 3, lower) are for validation needs, with a consideration of scientific importance; a bracket indicates routine data are likely to provide significant/sufficient validation. *Correlative data sources and opportunities:* column **S** is for satellite data: ++ = sufficient/significant amount, + = moderate amount (some extra efforts may be needed), **-** = small amount or poorly matched (without extra efforts, proper validation cannot be performed); column **G** is for ground-based data, including sonde networks. Column **B** (when filled in) represents a need/desire for balloon correlative data; column **A** is for a similar need/desire for aircraft correlative data (troposphere).

Parameter	Priority	OMI	TES	S	G	B	A	Comments
NO_2	1	C		+	+			Few correlative non-twilight ground-based data. Ground-based correlative data under polluted conditions needed, since troposphere dominates. Diurnal effects are an issue, see also Table I.2.
NO_2 (tropospheric)	1	$C_{trop}^{(1)}$		+	-	X	X	Ground-based (or other) campaign correlative data under polluted conditions needed. Main satellite correlative data: SCIAMACHY (nadir-viewing mode).
O_3	[1]	C	C $^{(a)}$	++	+			Sufficient amount of ground-based correlative data expected, see also Table I.2.
O_3 (tropospheric)	1	$C_{trop}^{(1)}$		+	+	X	X	Campaign efforts for validation of horizontal variability needed.
HCHO	2	C		+	-			Campaign efforts for ground-based column data needed (no routine ground-based correlative data sources). GOME also measures HCHO.
OClO	2	C		+	-			Few correlative non-twilight ground-based data. Diurnal effects are an issue.
BrO	2	C		+	-			Few correlative non-twilight ground-based data. Diurnal effects are an issue.
SO_2 (volcanic)	1	C	C $^{(1)}$	n/a	n/a			High priority if large volcanic eruption occurs.
SO_2 (background)	3	C	C $^{(1)}$	n/a	n/a			Under background conditions, no sensitivity, or high need for validation
UV fluxes, UV-B	2	•						Ground-based and airborne validation activities needed

(1) Not a standard product, at least initially (requires more time/research).

(a) Integrated column from TES profile.

III.4 Other Issues and Plans for Validation

There is a need for correlative surface albedo data (for OMI) and infrared surface emissivity (for TES). Raw radiance data from satellite instruments covering Aura wavelengths (e.g., GOME, SCIAMACHY, UARS MLS, ODIN/SMR, ASTER) can be used to perform consistency checks with Aura Level 1 data. The AES experiment will provide surface emissivity and near surface radiances for TES.

III.5 Ground-based Networks

Several ground-based networks (ozonesondes, Brewer/Dobson and Umkehr sites, radiosondes, NDSC, ARM, AERONET, and others) should provide accurate information about stratospheric and tropospheric profiles, and column densities for some of the constituents measured by Aura, as well as aerosol and cloud information (see Table 5.3). Such networks offer the best means for long-term validation of data from Aura and other satellites.

III.6 Other Satellite Data

Satellite measurements of stratospheric constituents expected during the Aura timeframe are given in Table 5.2 of this document. Observations that are validated prior to Aura launch will be useful for Aura validation. Data sets most likely to be useful for initial Aura validation studies will come from satellites launched ~2 years or more prior to Aura since the validation process, including reprocessing, can take years. Analyses of satellite-satellite comparisons can often point to certain problems beyond any systematic disagreements in absolute values.

Aura will follow Aqua by fifteen minutes in nearly the same orbit plane. The MLS instrument will make limb measurements 7.5 minutes behind the Aqua nadir point where AIRS and MODIS measure. This close formation will allow the water vapor measurements from AIRS and the cloud screening from MODIS to provide information for Aura instruments. Near the time of the Aura launch, the ESSP CloudSat and ESSP3 (PICASSO-CENA) missions will also be launched into the Aura/Aqua orbit plane; these satellites will follow Aqua by about 1 minute (and will be about 14 minutes ahead of Aura). The ESSP3 mission will make aerosol and cloud height measurements that will be especially useful to OMI and HIRDLS. In a similar fashion, measurements from other relevant correlative satellite programs should be exploited as much as possible.

III.7 Balloon Flights

Measurements of stratospheric profiles from balloon platforms are the only means to get high vertical resolution profiles for most constituents in the mid- to upper stratosphere (Table I.1). A series of flights at 2 or more latitudes over a 2-3 year period is viewed as a minimum need. High latitude campaigns using balloons are needed to provide profiles under the perturbed conditions of polar winter/spring. In situ or emission data are preferable to occultation data for species with significant diurnal variation (and potential variation along the line-of-sight) such as NO and NO_2, for optimal comparison with the Aura measurements; clearly, coordination with Aura overpasses becomes even more important in these cases. Measurements of tropospheric profiles from balloon platforms are needed, especially for tropospheric and lower stratospheric NO_2 and ozone in polluted areas.

III.8 Campaigns

Campaigns involve coordinated deployment of aircraft, balloon and ground based platforms to address scientific questions concerning key issues in atmospheric chemistry and dynamics. Such campaigns to study stratospheric phenomena have been carried out since the mid-1980's. The instrument payload used in those campaigns has been made more complete, and now measures many quantities of stratospheric interest. These data, combined with satellite information, have been utilized to well characterize atmospheric phenomena. For example, winter polar expeditions (e.g., AAOE, AASE I, AASE II, SOLVE, THESEO) have made repeated measurements within and near the polar vortex. These data, combined with continuing ground based measurements in the polar region, suggest that while limited focused measurements in these regions are appropriate for validation, major campaigns need not be developed to recharacterize those regions. However, the tropical upper troposphere and lower stratosphere have not been so completely characterized as the winter polar stratosphere. Although field campaigns to measure tropospheric quantities have taken place in the 1990's, there are no global databases for most tropospheric constituents. Validation activities for tropospheric data are necessary over a broad range of latitudes and seasons (see Section 5.2.3.1.3 and Table 5.4).

Such campaigns are being planned, with the additional requirement to fulfill specific Aura validation requirements. Themes being used to develop campaigns (section 5.2.3.5) have been identified in the context of the Aura scientific objectives (section 2) and the validation needs of Aura as presented in section 5. Descriptions of three missions are provided in Appendix 7C. The Tropical Composition and Climate Experiment (TC^3) is a multi-year, multi-sensor deployment with the goals of defining the chemical boundary condition for the stratosphere and the response of the atmospheric hydrological cycle to climate change. Two missions, the Intercontinental Chemical Transport Experiment (INTEX) and the Large-Scale Biosphere-Atmosphere Experiment in Amazonia focus on tropospheric chemistry issues. It is probably not possible to meet all the Aura needs of latitudinal and seasonal coverage for aircraft and balloon observations within the scope of these large campaigns.

III.9 Lower Stratospheric and Tropospheric Measurements for Aura Validation

Validation of Aura data in the lower stratosphere and troposphere is challenging. The validation strategy must take into account the geophysical variability of the region, large vertical gradients for constituents such as H_2O, O_3, CO, and limitations due to retrieval physics that reduce the precision of retrieved quantities. For some of the Aura products (ozone, water vapor up to ~ 150 hPa, and aerosols), ground-based networks provide sufficient data (in certain places) for statistical comparisons. Aircraft underflights of the satellite footprint can provide horizontal validation and scientific information that ground-based or balloon-borne measurements generally cannot. For limb measurements, coincidence between a satellite overpass and an aircraft flight is always limited because a satellite measurement is instantaneous compared with the several hours required for an aircraft to explore a satellite footprint. A high priority in exploration of the satellite footprint is the along-track gradient since this gradient has the greatest impact on the retrieval algorithm for limb measurements (ahead of or behind the satellite). For nadir-viewing instruments, with relatively small footprints, aircraft measurements have the additional advantage of providing many correlative measurements spaced closely together, which boosts the statistical robustness of the intercomparison and provides a handle on horizontal variability.

As discussed in sections 5.2.3 and 5.2.3.1.3, major tropospheric aircraft campaigns are limited in spatial and temporal coverage, and will probably not meet the requirements for TES validation summarized in Table 5.4. For the tropospheric observations that are the primary science products of TES, for the tropospheric and lower stratospheric observations from HIRDLS and MLS, and for the tropospheric column measurements of OMI, such campaigns will have to be supplemented by smaller, targeted aircraft campaigns that address remaining specific needs.

III.10 Models

After launch, fields from model simulations will be used for comparisons with measurements of all constituents, but especially for those measurements that are noisy and must be spatially and temporally averaged to have geophysical meaning. Assimilation techniques and techniques such as following parcel trajectories will also be utilized.

EOS Aura Science Data Validation Plan

Table of Contents

EOS AURA SCIENCE DATA VALIDATION PLAN

1 Introduction

1.1 Document History

Table 1.1. Document history

Version	Date	Comments	Coordinator/point of contact
0.1	Mar. 14, 2000	Initial draft and plan outline. Focus on section for correlative data needs and plans.	Lucien Froidevaux/JPL lucien@mls.jpl.nasa.gov
0.2	May 10, 2000	Updated draft and plan outline. Includes additional inputs from instrument teams + product- by-product discussion.	Lucien Froidevaux/JPL
0.4	June 2, 2000	Expanded Introduction. Added MLS inputs (for most of sections 2,3,4,5). Added OMI inputs (for most sections) + some OMI comments about the overall Plan (others to be discussed later). [Note: V0.3 was brief internal version for MLS/OMI iterations]	Lucien Froidevaux/JPL
0.5	Aug. 7, 2000	General clean-up & section renumbering. Added inputs from all teams, and Figure on instrument coverage overlap (2.2.5). A few "holes" remain (see "TBUpdated"). Campaign choices and ensuring that we can get sufficient correlative data for all Aura products viewed as main remaining planning issues.	Lucien Froidevaux/JPL Anne Douglass/GSFC douglass@persephone.gsfc.nasa.gov
0.6	Oct. 11, 2000	Added CH_3CN as MLS product. Updated most of remaining sections (and Appendix) except for campaign issues.	Lucien Froidevaux/JPL Anne Douglass/GSFC
0.9	Mar. 31,2001	Added campaign sections; include priorities as developed during Fall, 2000 meeting.	Lucien Froidevaux/JPL Anne Douglass/GSFC
1.0	July 12, 2001	Incorporated final team inputs on priorities, requirements + minor changes.	Lucien Froidevaux/JPL Anne Douglass/GSFC

1.2 Validation Working Group and Contributors

The Earth Observing System (EOS) Aura mission Validation Working Group has official representation from each of the four instruments aboard Aura: the High Resolution Dynamics Limb Sounder (HIRDLS), the Microwave Limb Sounder (MLS), the Tropospheric Emission Spectrometer (TES), and the Ozone Monitoring Instrument (OMI). The official representatives from each instrument team are listed below; they, along with the team principal investigators (and other team members) are responsible for putting this validation plan together.

Name	Affiliation	Coordinates
Douglas Kinnison	HIRDLS	dkin@ucar.edu
Lucien Froidevaux	MLS	lucien@mls.jpl.nasa.gov
Ellen Brinksma	OMI	brinksma@knmi.nl
David Rider	TES	david.m.rider@jpl.nasa.gov

Since validation of science data includes a variety of activities and is crucial for producing reliable scientific information about the atmosphere, an increasing number of scientists (probably almost everyone on each of the instrument science teams) is expected to become involved in this process as time gets closer to launch, and of course, after launch. In addition, the oversight and inputs of the Aura Project, as well as the EOS Planning Office (Dave Starr) and NASA Headquarters are/were clearly an important part of this planning and coordination process as well.

Other contributors to this document are listed below:

Mark Schoeberl	(Aura Project Scientist)
Anne Douglass	(Aura Project Deputy Scientist; co-chair of Valid. Working Group)
Ernie Hilsenrath	(Aura Project Deputy Scientist; OMI co-PI)

John Gille	(HIRDLS co-PI)
John Barnett	(HIRDLS co-PI)
Mike Coffey	(HIRDLS team)
David Edwards	(HIRDLS team)
Alyn Lambert	(HIRDLS team)
William Mankin	(HIRDLS team)
Steven Massie	(HIRDLS team and Chair of Aerosols Working Group)
Ken Stone	(HIRDLS team)

Joe Waters	(MLS PI)
Mark Filipiak	(MLS team)
Bob Harwood	(MLS team; UK PI for MLS)
Nathaniel Livesey	(MLS team and Chair of Algorithms Working Group)
Hugh Pumphrey	(MLS team)
Michelle Santee	(MLS team)
Bill Read	(MLS team)
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Gilbert Leppelmeier (OMI co-PI)
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Reinhard Beer (TES PI)
AnnMarie Eldering (TES team)
Daniel Jacob (TES team)
Jennifer Logan (TES team)
Stanley Sander (TES team)
Helen Worden (TES team)

Brian Johnson (formerly with HIRDLS, as Validation Working Group Rep.)
Stuart McDermid
Lynn Sparling
Geoffrey Toon
Owen Toon

1.3 Other Relevant Documents and Publications

There are several other documents and websites that offer more information about EOS, the Aura Project, and individual Aura instruments, requirements, and the associated plans for algorithms and data processing.

The main ones (of some relevance to validation) are listed below; full references for open literature publications are given in the "References" section at the end of this document.

EOS and Aura

- "1999 EOS Reference Handbook"
- EOS website: http://eos.nasa.gov/
- Aura website: http://eos-aura.gsfc.nasa.gov/

HIRDLS

These HIRDLS documents may be found on the HIRDLS website: http://www.eos.ucar.edu/hirdls/

- "HIRDLS Algorithm Theoretical Basis Document (Level 0-1)," R. Wells et al., SW-HIR-168, October 1999.
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1.4 Document Goals and Approach

This plan should focus and stimulate the large amount of work required, before and after launch, for the successful completion of the various activities relating to validation of the Aura mission science data. This plan concerns Level 2 data, since Level 1 data are quite specific to each instrument. Since there is significant overlap among the atmospheric measurements planned by the four instruments aboard the Aura satellite, an overall Aura Validation Plan is beneficial to all the teams involved. This does not preclude separate written plans for each instrument, especially if additional details are to be found in these plans. This document also includes a brief description of validation-related activities that are necessary for the broad validation process.

Section 1 of this document contains an introduction. Section 2 summarizes the scientific objectives of the Aura mission, and the instrument and measurement characteristics for the four instruments. Details of the measurement techniques are found in Appendix A. The science data products for each instrument are presented in section 3, along with expected uncertainties in these products. Section 4 concerns pre-launch validation activities, including summary plans for instrument calibration and retrieval algorithm testing, and identification of needs for additional or improved spectroscopic data and other data bases. Section 5 concerns the plans for post launch activities relating to validation. Section 5.1 discusses each instrument team's plans for post-launch data quality assessment (other than the correlative geophysical data comparison and related modeling efforts). Section 5.2 describes various correlative data sources for comparison with Aura measurements, and attempts to provide a path to optimize the validation and science returns of the combined measurements (from aircraft, balloon, and other campaigns, as well as more "routine" measurements from the ground or from space). This section is a primary focus before launch, because of the time needed to prepare for campaigns and plan for correlative data in support of Aura validation.

More specific plans and detailed implementation issues for correlative studies will be developed after specific programs and proposals for measurements have been accepted in support of these validation activities.

1.5 Validation Goals

The EOS Validation Program defines validation as "the process of assessing by independent means the uncertainties of the data products derived from the system outputs." An end-to-end pre-launch understanding and characterization of the instrument, algorithms and databases that will be used to generate data products and their uncertainties from the measurements are important. This includes algorithm testing, pre-launch, and validation, post-launch, and should be largely covered by the calibration documents and various ATBDs and follow-up documents. After launch, a series of validation activities ranging from calibration checks ("calibration") to comparisons of retrieved geophysical products with independent measurements of similar parameters ("validation") are needed to ascertain the quality of the data products.

1.6 Overview of Validation Plans

The pre-launch and post-launch activities planned for the Aura data towards the overall validation goals (which include calibration) should include the following important steps:

- *Characterization and calibration of the instruments*

Separate documents are planned to describe plans and results of this activity for each one of the Aura instruments (pre-launch and post-launch).

- *Algorithm testing*

  This important activity provides confidence in the retrieval algorithms, including both forward and inverse models, based on simulations, and comparisons between different techniques and/or software programs. This activity also includes reviews and updates of the Algorithm Theoretical Basis Documents (ATBDs) for each of the Aura instruments (see references mentioned in section 1.3 above).
- *Understanding of spectroscopic data and uncertainties*

  Spectroscopic data are an important external input with significant impact on the accuracy of retrieved geophysical products; some prioritized needs for improvements in this database are outlined in this document, and were also outlined in a NASA Research Announcement in support of validation for Aqua and Aura.
- *Characterization of expected measurement uncertainties*

  This involves retrieval simulations and sensitivity studies. Uncertainty estimates based on expected measurement noise are given here. Accuracy estimates will also be produced. Refinements of precision and accuracy estimates will continue through launch and beyond, since these estimates depend on the knowledge of instrument parameters and calibration, as well as spectroscopy. Establishing the validity of these estimates is a main goal of the validation activities after launch.
- *Careful inspection of incoming data*

  This involves the generation of analysis software and a manageable number of routine analysis products.
- *Examination of radiance residuals*

  This can point to radiance closure problems and their potential sources.
- *Comparisons of same measurements from different spectral bands*

  When this kind of analysis is possible, it serves as a consistency check.
- *Comparisons with climatology*
- *Intercomparisons between Aura instrument results*
- *Comparisons with correlative data*

  This is a crucial part of the validation process, involving "routine" measurements (e.g., ground-based, sonde, aircraft, other satellites), as well as measurements from specific campaigns (e.g., balloon and aircraft).
- *The use of atmospheric modeling and related methods for validation*

Each of the above activities will involve a significant commitment of resources; more details and references regarding the plans for each activity are given later in this document.

An overview of the main validation elements is presented in the schematic below (Fig. 1.1), where the importance of a variety of post-launch correlative data sets is illustrated. Aircraft and balloon campaigns need to be planned well ahead of launch, since it takes significantly more than a year to plan for such campaigns. In the following schematic "Calibration" includes the spectroscopic database and other relevant databases. Modeling includes the atmospheric modeling needed to simulate the measurements (the 'forward model'), retrieval algorithms (the 'inverse model'), and models used for comparisons with the retrieved geophysical products, data assimilation models or those used for trajectory mapping studies.

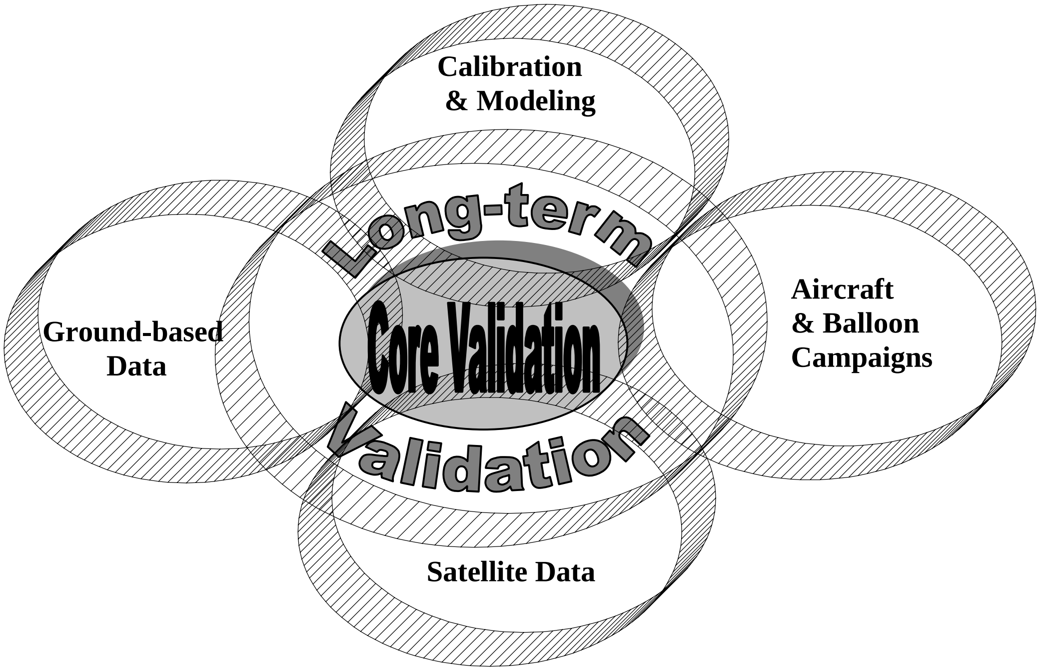


Fig. 1.1. Schematic Description of the Validation Elements.

1.7 Success Criteria

Successful validation of geophysical data products requires either that uncertainty estimates for the geophysical products have been shown to hold, based on independent comparisons with similar high quality data products that have already been validated themselves, or that the discrepancies between such comparisons have been understood and explained. At the completion of the validation efforts, a data user should have enough information to understand the data quality, in terms of precision and accuracy, as well as spatial/temporal variations in these quality attributes.

The conditions for success should include a reasonable timetable within which proper assessments of the data can be made, in order to provide timely validated products to the scientific community. This also requires sufficient planning for comparisons and validation, and the realization that this task should involve a significant group of scientists and support personnel both before and after launch.

2 The EOS Aura Mission

2.1 Scientific Objectives

2.1.1 Overview

Each of the four Aura instruments has scientific goals, described in the next 4 sub-sections, and targets specific measurement products to meet these goals (section 3). The measurement suite is broad, and will thus provide information to the science goals even as the science goals themselves evolve. There is both overlap and synergy among the measurement suites of the four instruments, and there is overlap among their science goals. Employing complementary data from each of the four Aura instruments, in conjunction with other data and theoretical analyses, will ultimately provide the most powerful way to accomplish the overall scientific objectives of the Aura mission.

The top-level objective is to resolve the following primary science questions:

- **Is the ozone layer changing as expected?**

- **Do we understand the transport of gases within the stratosphere and between the stratosphere and troposphere?**

- **What are the sources and distributions of tropospheric pollutants?**

- **What are the roles of upper tropospheric water vapor, aerosols, and ozone in climate change?**

2.1.2 HIRDLS Objectives

HIRDLS will provide observations of temperature, ozone, water vapor, eight other trace gases and aerosol or cloud parameters with horizontal and vertical resolution that is unprecedented in a global data set (section 3.1.2). The horizontal (longitudinal and latitudinal) resolution of 100-500 km, coupled with vertical resolution ≤ 1 km, is sufficient to resolve many structures and variations such as those around the tropopause and associated with internal barriers in the atmosphere. The vertical range extends from the upper troposphere to the mesosphere. These characteristics of HIRDLS observations are expected to be of major importance in reaching the primary Aura science objectives.

Eight principal scientific objectives have been identified as proposed foci for investigations for which the HIRDLS Science Team intends to use the data. These are:

1. To better understand the fluxes of mass and chemical constituents (including greenhouse gases and aerosols) that affect the dynamics and composition of the troposphere, stratosphere, mesosphere, and thermosphere and link these regions together.
2. To understand the chemical processing, transport, and irreversible mixing of trace constituents in the middle atmosphere, including the chemical and dynamical processes responsible for creating springtime ozone depletions in the Antarctic and Arctic.
3. To understand the momentum, energy, and potential vorticity balances of the middle atmosphere, by extending global observations to smaller horizontal and vertical scales than has previously been possible. These processes are believed to be fundamentally important to the determination of some large-scale characteristics and are thought to cause irreversible chemical mixing.
4. To obtain climatologies of upper tropospheric, stratospheric, and mesospheric quantities, in particular, profiles of temperature, ozone, several radiatively active gases, aerosol, gravity wave activity and cloud top heights. Seasonal, interannual, and long-term trends will be

obtainable because of the five-year measurement sequence that will be provided by each Earth Observing System (EOS) instrument, combined with pre-EOS measurements and future EOS observations.

5. To provide data to evaluate and improve numerical models of the atmosphere, in order to gain confidence in their ability to predict climate change. These simulations are critically dependent on the treatment of horizontal and vertical scales that are much finer than those currently observed.
6. To improve the understanding of tropospheric chemistry through the use of temperature and constituent retrievals that extend into the upper troposphere, under favorable conditions. The combination of these observations with observations from other EOS instruments, and with chemical models, will yield information about the oxidation capacity of the atmosphere.
7. To improve the understanding of stratospheric and tropospheric aerosols and clouds by acquiring long-term high-resolution observations of their nature and distribution. Aerosols and polar stratospheric clouds are now known to play essential roles in the depletion of ozone in the lower stratosphere, and subvisible cirrus clouds in the upper troposphere significantly impact the radiative heating and cooling of the atmosphere.
8. To improve tropospheric temperature and water vapor profiles and cloud top height data that are used for climate and weather forecasting, by combining high vertical resolution limb data with data from operational nadir sounders such as AIRS and AMSU.

The functional requirements for the HIRDLS instrument have been determined by considering the data quality that is necessary to produce useful results from these key studies.

The relationships of these objectives to the Aura objectives are indicated below.

Is the ozone layer changing as expected?

The period at the beginning of the 21st century offers a unique opportunity to study stratospheric chemistry at a period when the chlorine loading is near a maximum. Under these circumstances it is crucial to monitor the ozone distribution, and quantify the influence of trends in the species that interact to produce or destroy it, as well as the temperature that affects reaction rates. HIRDLS species, especially when combined with MLS measurements, will allow detailed constraints of the chemical balances. Quantitative studies will also require careful calculation of dynamical effects. The HIRDLS high-resolution observations are uniquely suited to this application. Detailed measurements of the seasonal and spatial variations will provide tests of stratospheric photochemical processes and clarify mechanisms that transport ozone from the lowermost stratosphere to the troposphere.

Note that HIRDLS high-resolution ozone profiles may be integrated to yield the stratospheric column amount, which may be subtracted from the OMI total column to yield the tropospheric column at all latitudes.

Do we understand the transport of gases within the stratosphere and between the stratosphere and troposphere?

In the overworld, at potential temperatures above ≈ 400K, much of the transport is believed to be due to the working of the residual circulation, and planetary scales are most important. However, much mixing takes place in the surf zones, where smaller scales are generated by breaking planetary waves. In addition, smaller scales are associated with motions across vortex boundaries and at the tropical barriers. HIRDLS capabilities should significantly improve our understanding of these transports.

Such motions are also important to the Upper Troposphere/Lower Stratosphere (UT/LS) region. In mid-latitudes synoptic scale waves can penetrate into the low stratosphere, and are expected to be important in isentropic transports between the tropical troposphere and lowermost stratosphere. In the tropics, small vertical scales are associated with the sharp tropopause, as well as thin layers of cirrus, and some global scale waves.

Effects of gravity waves are also believed to be important, and significant parts of the gravity wave spectrum should be observable by HIRDLS.

What are the sources and distributions of tropospheric pollutants?

HIRDLS observations will extend down into the upper troposphere. They can contribute to this question by providing observations and understanding of the transports of stratospheric species, notably ozone and nitric acid, into the troposphere. Other upper tropospheric species of interest are water vapor (which with ozone is the classic source of hydroxyl radical), and nitrogen dioxide.

What are the roles of upper tropospheric water vapor, aerosols, and ozone in climate change?

UT/LS water vapor and ozone are critical gases in maintaining the earth's radiative balance. At this time their distributions in the UT/LS are not well known, and the mechanisms by which their distributions are maintained are not understood. In particular, the mechanism by which the stratosphere is dehydrated is still a subject of great speculation, over 50 years after Brewer's work. While some of the process may well be due to microphysical processes, which will not be observable from space, continuing measurements with the detail of those provided by HIRDLS should shed more details, and hopefully insight, on the "tape recorder" and other proposed mechanisms.

2.1.3 MLS Objectives

MLS will provide measurements of a broad suite of constituents in the upper troposphere and stratosphere (section 3.2.2). These observations are necessary to address the scientific objectives of the MLS investigation and three of the four overall objectives of the Aura mission.

Determining if stratospheric ozone is changing as expected

Solomon [1999] reviews the processes governing the ozone layer, its natural production and destruction, and the history of ozone depletion. MLS observations will make it possible to address a broad spectrum of questions concerning the future of the ozone layer as man-made chlorofluorocarbons decrease due to international regulation, but climate change continues due to growth in the atmospheric burdens of greenhouse gases. MLS observations will be used to quantify the following: a) trends in upper stratospheric constituents such as HCl; b) trends in temperature, water vapor, and nitric acid, which affect polar stratospheric cloud formation and depletion of lower stratospheric polar ozone; c) changes in stratospheric circulation and transport; d) the effect of volcanic eruptions on stratospheric ozone, if a major eruption takes place. MLS will provide the first extended global stratospheric observations of the hydroxyl radical, which participates in many aspects of stratospheric photochemistry, including catalytic ozone destruction, destruction of source gases, and production and destruction of reservoir species.

Helping understand ozone pollution in the upper troposphere

Ozone is a pollutant in the lower troposphere. In the upper troposphere it is important because its photolysis in the presence of water vapor is the primary source of hydroxyl radicals that are responsible for oxidative removal of many polluting trace gases. Simultaneous measurements of O_3 and tracers of air motion (CO and HCN) will provide new global information on the sources of tropospheric O_3 and its variability. EOS MLS will measure the stratospheric ozone column more accurately than was possible with UARS MLS, thus the tropospheric residual (the difference between the total column ozone, measured by another sensor and this stratospheric ozone column) will be better determined.

Improving knowledge of processes affecting climate variability

MLS will provide measurements of upper tropospheric water vapor, even in the presence of cirrus where observations by other techniques (infrared, visible, and ultraviolet) can be flawed. These measurements are especially valuable because of uncertainties in climate feedback mechanisms associated with upper tropospheric H_2O [e.g., Lindzen, 1990]. Simultaneous MLS measurements of water in both the vapor and ice phases, temperature, and tracers of air motion (CO and HCN) should provide new information on processes affecting formation of cirrus ice particles. This information will be used to understand forcings such as El Nino that affect climate variability on seasonal-to-interannual time scales. MLS temperature measurements complement those from infrared techniques in that they are not affected by variations in stratospheric aerosol content or CO_2.

2.1.4 TES Objectives

TES will contribute to the Aura science goals by observing the three-dimensional distribution of gases important to tropospheric chemistry. These observations (see section 3.3.2) will be used to study troposphere-biosphere interactions and troposphere-stratosphere exchange. TES will provide the first global view of the chemical state of the troposphere, focused on mapping the global distribution of tropospheric ozone and understanding the factors that control ozone concentrations. TES will observe: the distributions of tropospheric ozone and its precursors (carbon monoxide, nitrogen oxides, methane and other hydrocarbons); sources and sinks of species important to the generation of tropospheric and stratospheric aerosols; effluents from biomass burning and major industrial accidents. These observations are most important to the third and fourth Aura objectives.

Sources of tropospheric pollution

Ozone in surface air is toxic to humans, animals and vegetation. It is the principal harmful component of smog. Ozone is produced in the troposphere by photochemical oxidation of carbon monoxide and hydrocarbons in the presence of nitrogen oxides and water vapor. These ozone precursors have both natural and anthropogenic sources. The chemistry of ozone is tightly coupled to the atmospheric transport of both ozone and the precursors, thus the global TES measurements will provide essential information.

The role of ozone in climate change

Ozone in the middle and upper troposphere is an efficient greenhouse gas. Perturbation of ozone in this region results in heterogeneous radiative forcing with complicated implications for climate change.

2.1.5 OMI Objectives

The Ozone Monitoring Instrument (OMI) will contribute to the EOS Aura mission objectives for climate monitoring and atmospheric research by measuring ozone and other minor atmospheric constituents like NO_2, aerosols, surface UV, cloud parameters, and sulfur dioxide released from volcanoes (section 3.4.2). OMI will provide the continuation of the TOMS total ozone data record, and will contribute to the science questions in atmospheric research concerning the role of ozone in the climate system. OMI aims to deliver global, near-real time (NRT) ozone observations for assimilation in numerical weather prediction (NWP) models [Levelt et al., 2000a, 2000b; Veefkind et al., 2000].

Changes in stratospheric ozone

OMI will make important contributions to the monitoring of the chemical composition of the stratosphere, including the ozone layer and its variability, and the assessment of long-term trends in ozone. The most important OMI objectives are continuation of the TOMS and GOME total ozone records for monitoring the Antarctic ozone-hole and the ozone layer and to detect trends and continuation of the SBUV and GOME ozone profile measurements. OMI column measurements of BrO, OClO and NO_2 similar to GOME provide an integrated measure of seasonal and interannual changes in minor constituents that impact ozone. The OMI objectives place requirements on accuracy, frequency of observation, coverage, horizontal resolution and, where relevant, vertical resolution for each OMI data product. A summary of these requirements for each OMI data product is given in Table 3.8 (see section 3).

Tropospheric Pollution

For measurement of pollution in the troposphere, the main contributions of OMI include measurements of O_3 and NO_2 (tropospheric) columns, aerosol optical thickness, HCHO, SO_2, and dust column densities in plumes and surface UV radiation. Daily global measurements of O_3 and NO_2 with a high horizontal resolution will enable EOS-Aura to trace and follow tropospheric pollution on a regional scale.

Climate Change

OMI will contribute to important science questions in atmospheric research concerning the role of ozone in the climate system through continuation of the TOMS total ozone data record and by providing ozone profiles for the study of dynamical, chemical and radiative processes in the upper troposphere and stratosphere. OMI aerosol products and detection of clouds will also contribute to questions about climate change.

Other goals

OMI contributions to the area of operational meteorology include daily global ozone columns (13 x 24 km^2 ground pixel size) and daily global ozone profiles (13 x 48 km^2) in near-real time for use in numerical weather prediction models. OMI will provide UV-Index forecasts using near-real time ozone columns. Finally, OMI products can be used for hazard detection through detection of emissions from volcanic eruptions.

2.2 Instrument Characteristics

2.2.1 HIRDLS Characteristics

The HIRDLS measurement technique is described in Appendix A; HIRDLS measures infrared emission from the atmospheric limb (in narrow-band spectral channels from 6 to 18 μm) behind the Aura satellite.

2.2.1.1 HIRDLS Measurement Coverage and Observation Modes

The HIRDLS instrument is designed to be versatile in its ability to scan the instrument line-of-sight (LOS) in the vertical (elevation) over a wide range of horizontal (azimuth) positions. This permits observing both poles, as well as dense coverage of measured profiles. The LOS azimuth position and both the elevation scan rate and range can be individually commanded. Observing modes, i.e., standard elevation and azimuth scan patterns, are designed to address a range of scientific investigations and are briefly described in this section. The primary observing modes provide broad, contiguous global coverage. In addition to the standard modes, other viewing modes not currently planned can be developed as the need arises, for example to view interesting geophysical phenomena, or as part of special engineering testing. Operational use of special viewing modes will be limited by the desire to provide observational data that is spatially and temporally uniform over the life of the HIRDLS mission.

In the **Global Observing Mode**, the normal mode for scientific data collection, there will be 6 vertical scans separated by 5 degrees in the across-track direction (~ longitudinal direction) and 4 degrees along the satellite track (~ latitudinal direction). Each vertical scan covers about 3 degrees in elevation and will be completed in 10 seconds. The entire azimuth swath will be completed in approximately 66 seconds, covering a range of LOS azimuth angles from -21 to 43 degrees. In-flight radiometric calibration will be performed by viewing cold space above the atmospheric limb signal every elevation scan and by viewing an internal warm blackbody calibration source after every complete swath. Equal longitudinal spacing of profiles leads to progressively closer horizontal spacing of profiles along the longitudinal direction as the spacecraft moves poleward.

The **Alternative Global Observing Mode** provides vertical profiles with a fixed horizontal distance of 500 km between profiles in the across-track direction and 400 km along-track (see Figure 2.1).

The **Medium Resolution Observing Mode**, with a profile spacing of approximately 2.5x2 degrees, and the **High Resolution Observing Mode**, with a spacing of 1x1 degrees, provide finer horizontal spacing of profiles, but do not provide contiguous coverage from orbit to orbit. These modes are desirable for observing regions with strong horizontal gradients such as the polar vortex boundaries. In the Medium Resolution mode, the in-flight calibration target is viewed after every other azimuth swath maintaining the 66 second calibration period; this mode produces 3 vertical profiles per swath, each profile scan taking about 10 sec to be completed. In the High-resolution mode, there will be 2 vertical scans per swath and 3 swaths between views of the in-flight calibrator.

The **Tropopause Mode** would observe the upper troposphere and lower stratosphere with high horizontal and vertical spatial resolution, and high signal to noise. This is accomplished by a combination of three "short" vertical scans spanning only the altitude range of interest and a "long" scan that will include observations to high altitudes and a view of cold space for zero correction. Finally, a **Selected Targets Mode** would view certain fixed geographic locations to study, for example, volcanic eruptions, the formation of polar stratospheric clouds, and to facilitate comparisons with ground-based correlative data.

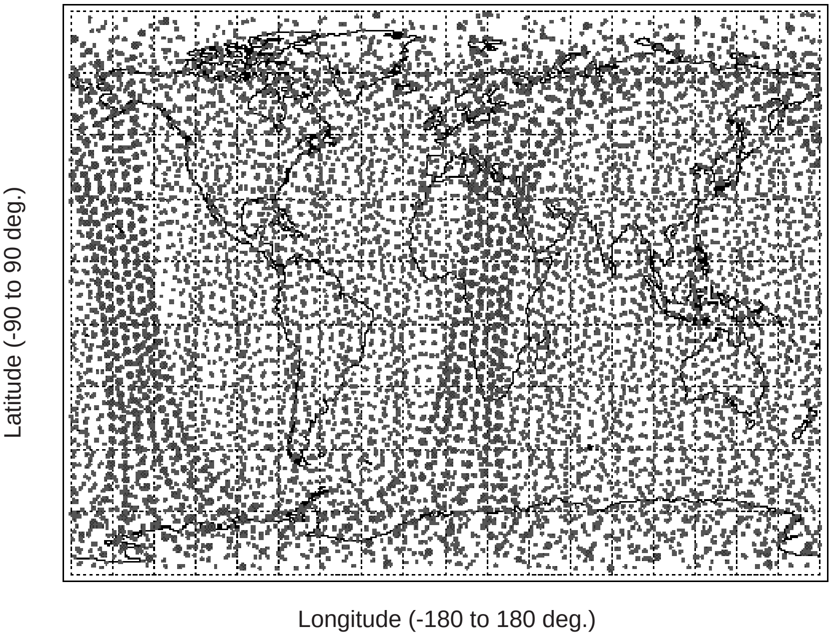


Figure 2.1. Tangent point locations of HIRDLS boresight for one day of observations in alternate global observing mode. Darker points show observations during a single orbit.

2.2.1.2 HIRDLS Measurement Resolution

As noted above, HIRDLS has been designed so that its field-of-view (FOV) can be stepped in azimuth several times during a science-observing mode scan pattern. The HIRDLS global mode observations will provide a nominal profile spacing of 400-500 km globally both along and across the orbital track. Special science-observing modes are available for which a local spacing of 100 km by 100 km can be achieved, however, these modes produce larger profile gaps in between successive orbital tracks.

The intrinsic vertical resolution is determined by the combination of limb geometry and the exponential falloff of atmospheric density. This results in most of the contribution to observed radiance arising from very near the tangent point, characterized by narrow limb weighting functions. The weighting functions from each of the spectral channels will be further broadened by the HIRDLS 1-km vertical FOV. By oversampling each FOV by a factor of 5, and with low noise, it is expected from retrieval simulations that vertical wavelengths of the order of 1.5 km and longer should be adequately reconstructed from HIRDLS limb radiance measurements.

The horizontal FOV is 10 km at the limb. However, there will be little or no information about horizontal gradients on this scale that can be resolved from HIRDLS observations.

The along-track horizontal resolution is determined by the radiative transfer process along the line-of-sight path which results in a rather broad horizontal weighting function and is limited to approximately 250-300 km. However, including the line-of-sight variations in the calculations could reduce this averaging length somewhat.

2.2.2 MLS Characteristics

The MLS measurement technique is described in Appendix A; MLS resolves microwave and sub-millimeter spectral lines from atmospheric limb emission ahead of the Aura satellite.

2.2.2.1 MLS Measurement Coverage and Observation Modes

The Aura orbit is sun-synchronous at 705 km altitude with 98^o inclination and 1:45 p.m. ascending equator-crossing time. MLS performs observations with the instrument fields-of-view scanning the limb in the orbit plane to provide 82^o N to 82^o S coverage. Limb scans for nominal operation are synchronized to the orbit (using the node-crossing signal from the spacecraft), with the number of scans per orbit an integer multiple of 4, and phased such that limb scan locations occur over the equator. This gives the same latitude sampling in northern and southern hemispheres, and on ascending and descending portions. MLS nominal operations have 240 limb scans/orbit to give 1.5^o (165 km) along-track separation between adjacent limb scans. Fig. 2.2 shows the measurement locations with this scan pattern for one 24-hour period.

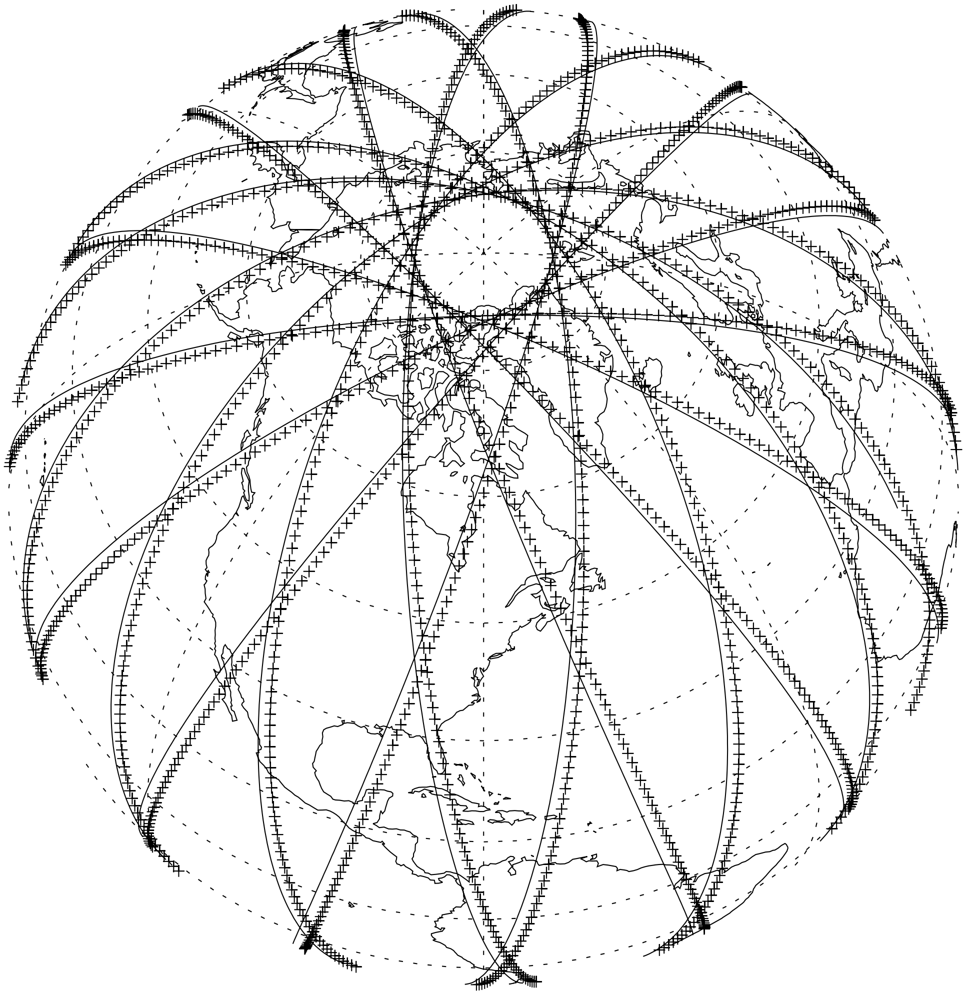


Figure 2.2. EOS MLS measurement locations for a 24 hour period. Each cross gives the location of the tangent points for individual limb scans. The continuous line is the sub-orbital track, which is slightly displaced from the tangent points because of Earth's rotation during the time in which the satellite moves forward to the tangent point latitude. The ascending portions of the orbit are those with the southeast-northwest tilt. Daily coverage at high latitudes in the Southern Hemisphere is analogous to that of the Northern Hemisphere shown here.

The nominal profile for individual limb scans is shown in Figure 2.3, and has repeat period (24.7s) that is 1/240th of the orbital period. The scan range is 15 to 62.5 km for the THz radiometer, and 2.5 to 62.5 km for the GHz radiometers that provide measurements to lower altitudes in the troposphere. This scan spends more time in the lower stratosphere and, for the GHz radiometers, in the upper troposphere, to emphasize these atmospheric regions which are currently of great scientific interest. The scan will be performed continuously (i.e., non-stepped), and the 1/6 s instrument integration time provides radiance measurements every ~0.3 km in the vertical in the upper troposphere and lower stratosphere and every ~1 km in the middle and upper stratosphere. Alternative scan programs will be used occasionally to provide measurements at higher altitudes in the mesosphere and in the lower thermosphere for some measurements. MLS observes in the direction of orbital motion (*forward),* and the limb is scanned in an *upward* direction to give an observation path tangent point locus that is nearly vertical. The tangent points at greater heights are closer to the satellite, but in the Earth frame of reference this is compensated by the satellite's forward motion. The horizontal deviation of the tangent point locus from a vertical line is approximately ±20 km (tilting forward below ~25 km tangent height, and backward above ~25 km tangent height) over the complete scan range for the nominal scan pattern described above [see Livesey and Wu, 1999, for a more detailed schematic of the tangent point loci].

It is expected that all measurements will be performed simultaneously. The planned mode of operation is therefore a simple continuous scanning mode. In the event of power constraints, a time sharing strategy will be devised.

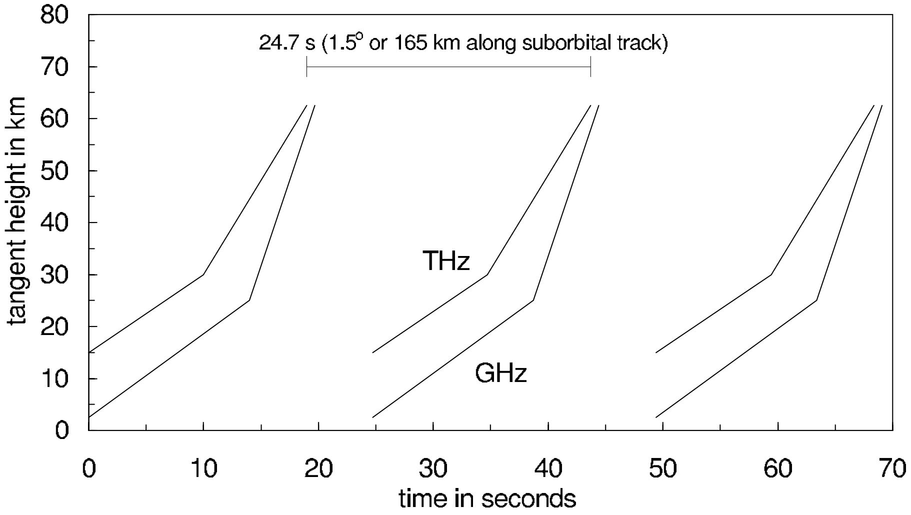


Figure 2.3. EOS MLS nominal operational scan. The curves give the height, at the tangent point, of the FOV boresight as a function of time. Radiometric calibration (observation of blackbody target and of cold space) and mirror retrace are performed during each gap. The scan is in the upward direction from lower to higher heights, causing the tangent point loci to be more vertical when plotted as a function of horizontal distance [Livesey and Wu, 1999]. The ~1 s difference between the end times of the THz and GHz scans is to reduce peak torque to the spacecraft when mirrors are moved more quickly through a larger angular range following the end of the limb scan. Refinements to this nominal scan are being considered, mainly to provide better coverage of the mesosphere, with negligible impact on the stratosphere and troposphere.

As the Aura orbit is sun-synchronous, MLS observations at a given latitude on either the ascending or descending portions of the orbit have the same local solar time throughout the mission. The local solar zenith angle at a given latitude and the boundaries between day and night portions of the orbit vary around an annual cycle, as shown in Figure 2.4.

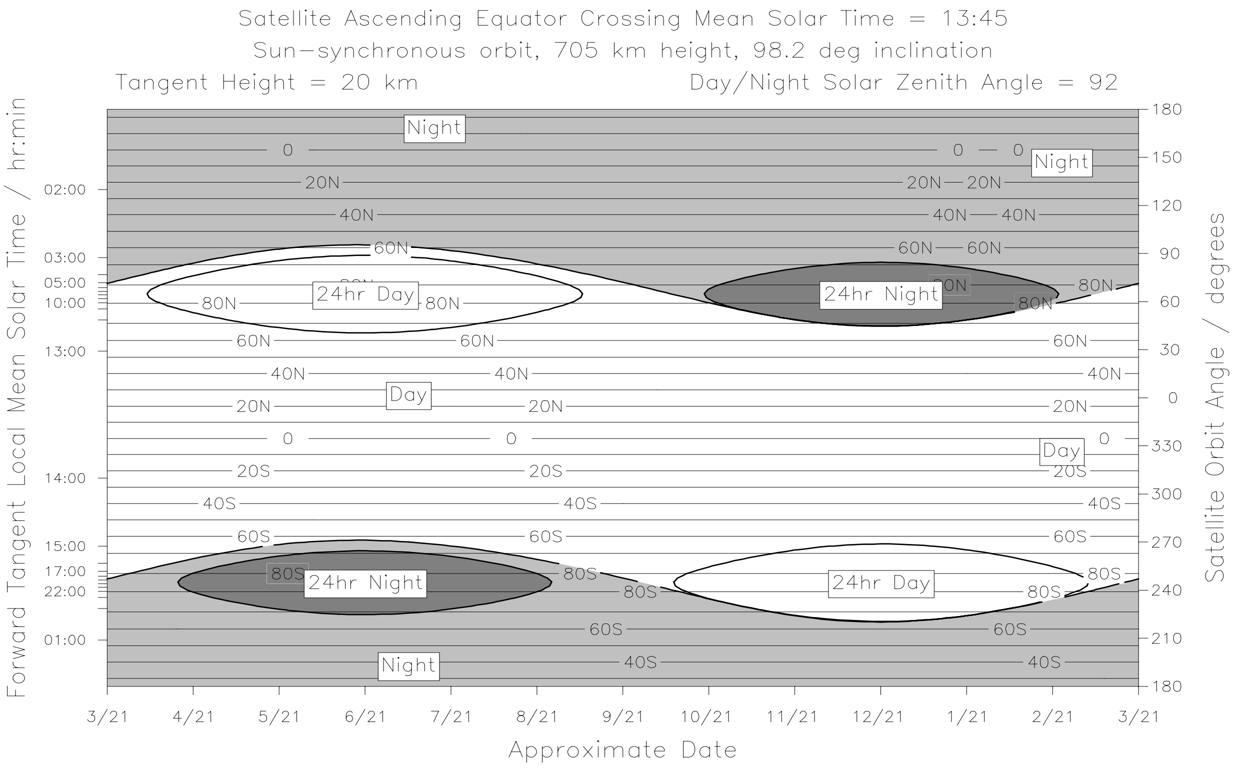


Figure 2.4. Variation, over an annual cycle, of the latitude range where MLS measurements are in day and in night. The horizontal axis gives the approximate date. The right hand vertical axis gives the orbit angle (defined as zero when the satellite is over the equator); the left hand vertical axis gives the corresponding local mean solar time at the (forward) tangent point of observations. Horizontal lines give the latitude of the tangent point, and the day-night boundary is defined as 92^o local solar zenith angle.

2.2.2.2 MLS Measurement Resolution

The vertical extent of the MLS FOV varies between 1.5 and 6.5 km. The finest vertical resolution for the MLS measurements is ~1.5 km, for 640 GHz radiometer data, based on full field-of-view width between half-power points; the FOV beamwidth is ~6.5 km for the 118 GHz data. The retrieval pressure grid for all MLS products has been chosen at 12 surfaces per decade change in pressure (with bottom surface at 1000 hPa), or about 1.3 km, in order to roughly match the best achievable resolution. There is always a compromise between vertical grid spacing and precision, with poorer precision obtained for a finer vertical grid [Filipiak, 1999]. This also means that stronger interdependence (anti-correlation) can be expected for adjacent surfaces, in the case of measurements having wider FOV (lower frequency). Based on the UARS MLS experience, useful profiles can be generated for a retrieval grid that is significantly finer than the FOV beamwidth. We plan to explore this in more detail as part of pre-launch simulations, so that enough information is made available after launch regarding the proper interpretation of MLS profiles and their assigned uncertainties (or error covariances).

The horizontal extent of the MLS FOV, perpendicular to the line-of-sight, varies between 2 and 13 km, for the various radiometers. Smearing (or averaging) of the atmosphere occurs along the line of sight over a distance of about 300 km, because of the sensitivity to radiative transfer along this path. Independent information from adjacent scans, separated by about 165 km, will help reduce this smearing effect if the retrieval for a given profile uses radiance information from more than one scan [Livesey and Wu, 1999; Livesey and Read, 2000].

2.2.3 TES Characteristics

The TES measurement technique is described in Appendix A; TES is a Fourier Transform spectrometer that measures infrared emission (3.3 to 15.4 µm) at high spectral resolution in both the nadir mode and the limb mode.

2.2.3.1 TES Measurement Coverage and Observation Modes

TES observes the atmosphere via a two-axis gimbaled pointing mirror, under control of a precision pointing system. The system provides views in a 45° half-angle cone about nadir, a view of the trailing limb directly behind the Aura satellite, a view of cold space and views of internal calibration sources. The range of viewing angles is illustrated in Figure 2.5. The system operates in a targeted mode for nadir measurements so that the area of observation remains fixed over the duration of a spectral scan. The detector array element footprints on the limb and on the surface are shown in Figure 2.6. The angular field-of-view of each detector array element is 0.75 mr x 7.5 mr. When observing the limb, the detector arrays view 16 contiguous altitudes in the troposphere and lower stratosphere (0-30 km) simultaneously. Each detector element views over an area of 2.3 km in altitude x 23 km cross track. For nadir observations 16 contiguous areas on the ground are viewed, each 0.53 km along track x 5.3 km cross track.

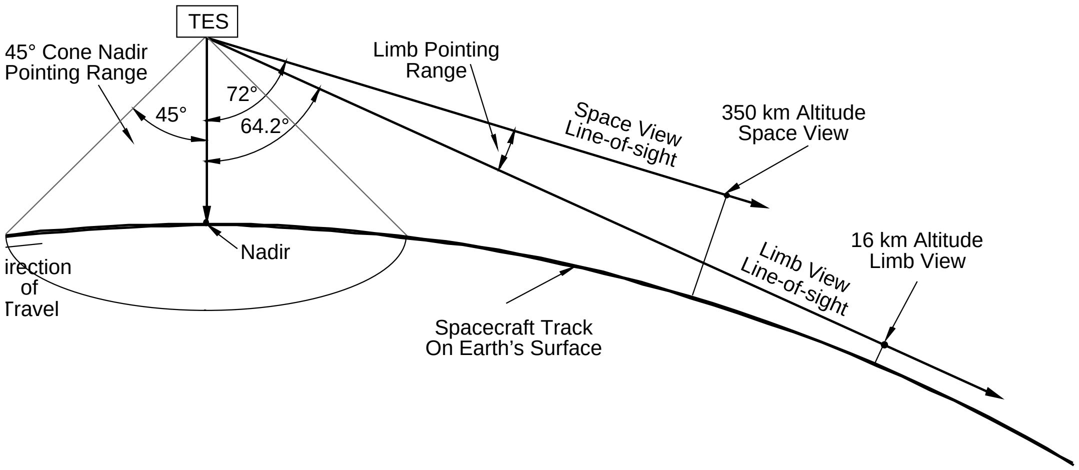


Figure 2.5. TES viewing geometry.

The pointing mirror, spectral resolution (0.1 cm^{-1} or 0.025 cm^{-1}) and suite of optical bandpasses in each of the four detector arrays are programmable, allowing great flexibility in the design of observations. For normal operations, the global survey mode, TES obtains data in a seven spectral scan sequence that covers about 5° of latitude. The sequence is: two calibration observations (a space view and a calibration source view) followed by two nadir observations and three limb observations. The sequence requires 81.2 seconds to complete, and is repeated continuously. In the Aura orbit (705 km altitude, sun-synchronous orbit, inclination = 98.21°, 1:45 pm equator crossing time, 99 min period), the along track distance traveled during the sequence is just under 5° or about 550 km. TES acquires 146 calibration and nadir spectra and 219 limb spectra in each of 64 detector array elements in each orbit. The current mission plan employs the global survey mode about half the time in a four day on, four day off cycle. Shorter duty cycles, as short as one day on and one day off, are under consideration.

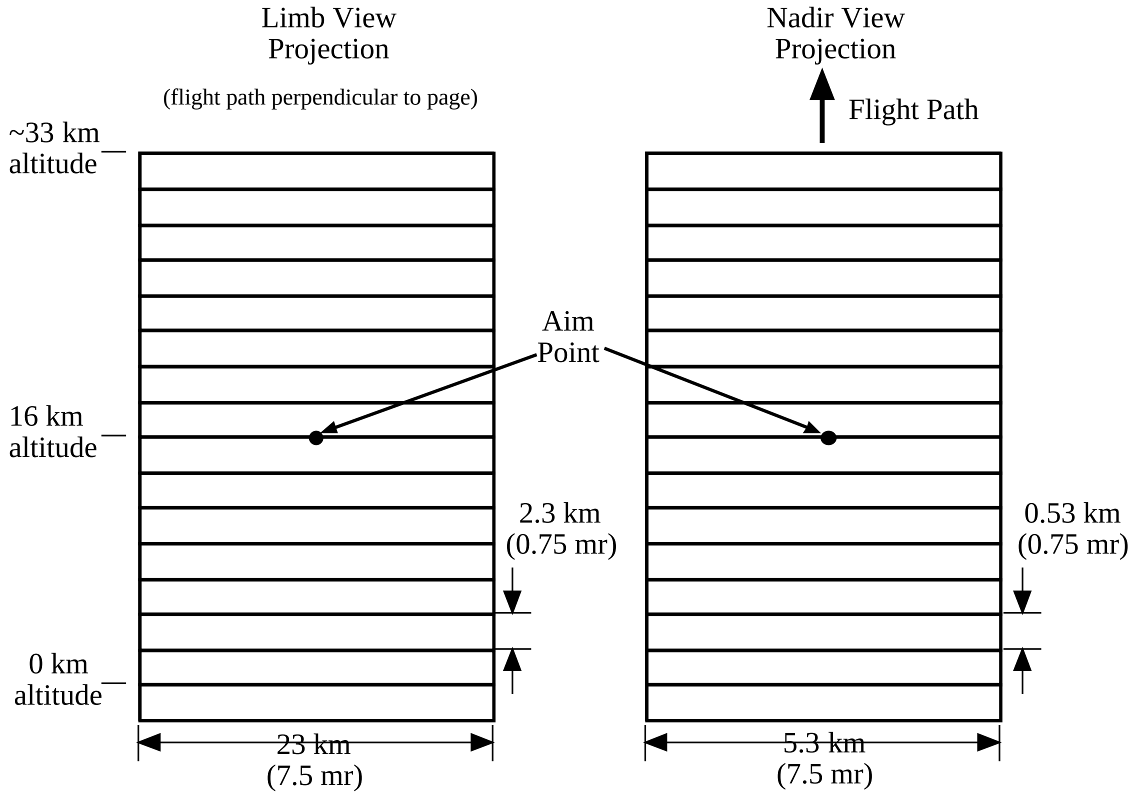


Figure 2.6. TES Fields-of-view projected onto the limb and the nadir surface.

The TES global survey mode observations are in-track so that the normal measurement latitudinal coverage is the 82N to 82S coverage of the Aura orbit spacecraft track. Aura orbit tracks over a one day period are shown in Figure 2.2. Forty five degree off-nadir views can extend this coverage by about a degree at each pole. Longitudinal coverage is also determined by the Aura orbit.

The pointing mirror target, filter mix, and spectral resolution are all programmable and allow the spatial and spectral coverage to be optimized for special observations, for example in support of validation campaigns, inter-instrument comparisons and targets of opportunity. A mode providing limb observations co-located with HIRDLS is a pre-programmed mode. This programmability allows, for example, concatenation of nadir observations both along-track and cross-track.

2.2.3.2 TES Measurement Resolution

Measurement resolution has many meanings, and depends on the viewing geometry, the signal-to-noise, the data level (e.g. profiles as opposed to maps and assimilated products), and on the vertical and spatial distribution of the detected species. The discussion here is limited to the vertical resolution and horizontal extent of single level 2 nadir and limb profiles of TES standard products.

In the limb, all radiances are measured with 16 contiguous 2.3 km vertical by 23 km horizontal fields-of-view. In the vertical, the radiative transfer process is also of importance and limits the vertical resolution of limb views to about half a scale height.

Combining these two factors, the TES retrieved limb profiles have a vertical resolution of 2.5 to 3.5 km. Radiative transfer completely determines the vertical resolution of nadir measurements and limits it to about a scale height. The TES profiles derived from nadir measurements have a vertical resolution of 4 to 6 km. When limb and nadir profiles are combined, the vertical resolution will vary with height. In round numbers the vertical resolution of profiles of TES standard products will be 4 to 6 km from the surface to approximately 10 km and about 3 km from 10 to 30 km.

Line-of-sight averaging, about 120 km, determines along-track horizontal extent of limb profiles while averaging over the FOV cross track dimension determines cross-track extent. The horizontal extent of a TES limb profile is 23 km cross-track x 120 km along-track. Field-of-view alone determines the horizontal extent of the nadir profiles. Standard product nadir profiles are averages of the 16 detector elements and have a horizontal extent of 5.3 km cross-track x 8.5 km along-track.

2.2.4 OMI Characteristics

The OMI measurement technique is described in Appendix A; OMI is a nadir-viewing wide-field imaging spectrometer measuring ultraviolet and visible backscattered solar radiation.

2.2.4.1 OMI Measurement Coverage and Observation Modes

The wide field of view of OMI (114°) yields a swath width of 2600 km at the altitude of the Aura satellite (705km). OMI uses 2 CCD detectors, one in the UV (270-365nm) and one in the VIS (350-500 nm) wavelength range. The UV wavelength range is divided in 2 channels: UV-1 (270-310 nm) and UV-2 (310-365 nm). One axis of the CCD is used for wavelength registration. The other is used for the swath direction (see Figure 2.7). Global coverage, except for small areas at the equator, is achieved in one day.

The nominal integration time of the CCD is 0.4 s. The data rate is decreased and S/N increased by onboard binning and co-adding of subsequent CCD images. The nominal co-addition time is 2 s. Using this co-addition time, for a swath of 2600 km, a nadir pixel size of 13×24 km^2 is possible for the VIS and UV-2 channels, and 13×48 km^2 for the UV-1 channel. This observation mode is called the *global observation mode* (in Figure 2.8 the global coverage of this mode is shown). Alternative modes (spatial zoom-in or spectral zoom-in) offer the possibility of smaller ground pixels at the expense of swath width or spectral range. An overview of the characteristics of each mode is given in Table 2.1.

Table 2.1. OMI swath width and nadir pixel size (along × across track) for different observation modes.

Observation mode	Swath width	Nadir ground pixel size	Spectral range	Application
Global mode				
UV-1	2600 km	13×48 km^2	270 – 310 nm	Global observation of all products
UV-2 & VIS	2600 km	13×24 km^2	310 – 500 nm	
Spatial zoom-in mode				
UV-1	2600 km	13×24 km^2	270 – 310 nm	Regional studies of all products
UV-2 & VIS	725 km	13×12 km^2	310 – 500 nm	
Spectral zoom-in mode				
UV	2600 km	13×12 km^2	306 – 364 nm	Global observation of some products
VIS	2600 km	13×12 km^2	350 – 432 nm	

Other observational modes are possible, due to flexibility in CCD read-out programming.

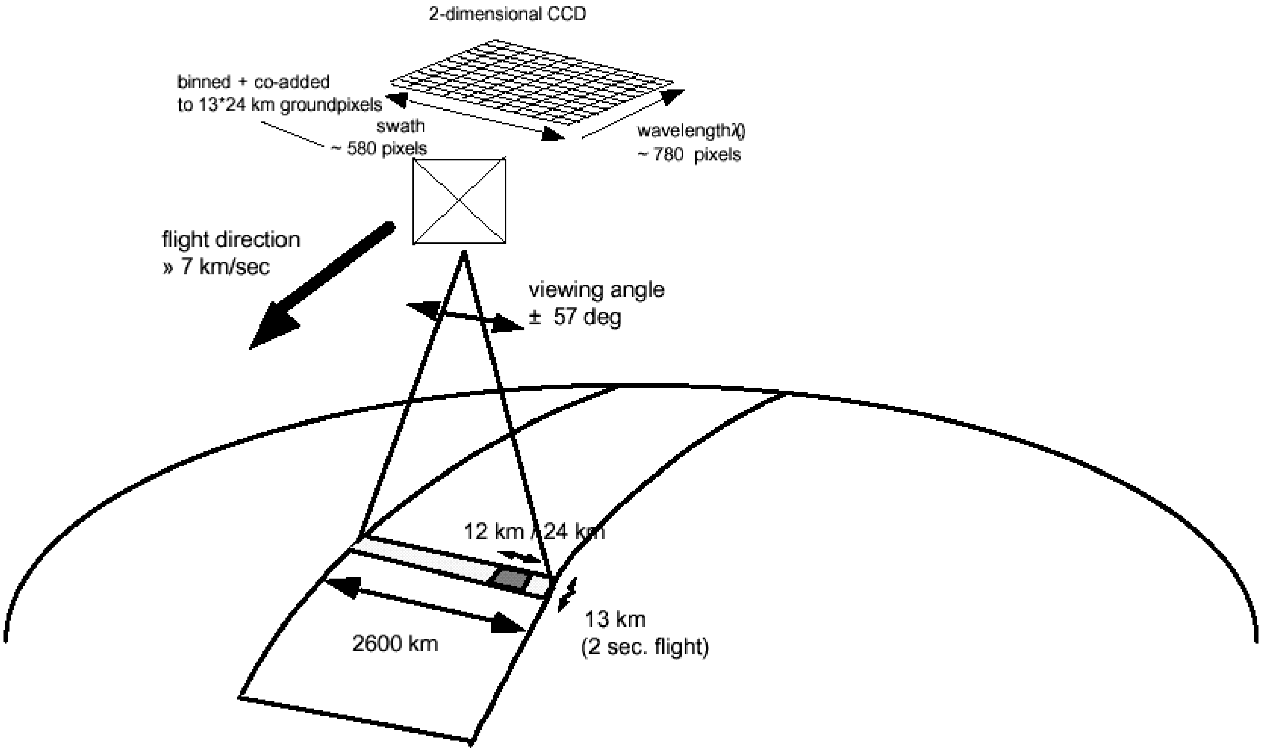


Fig. 2.7. OMI CCD measurement principle (© Fokker Space BV)

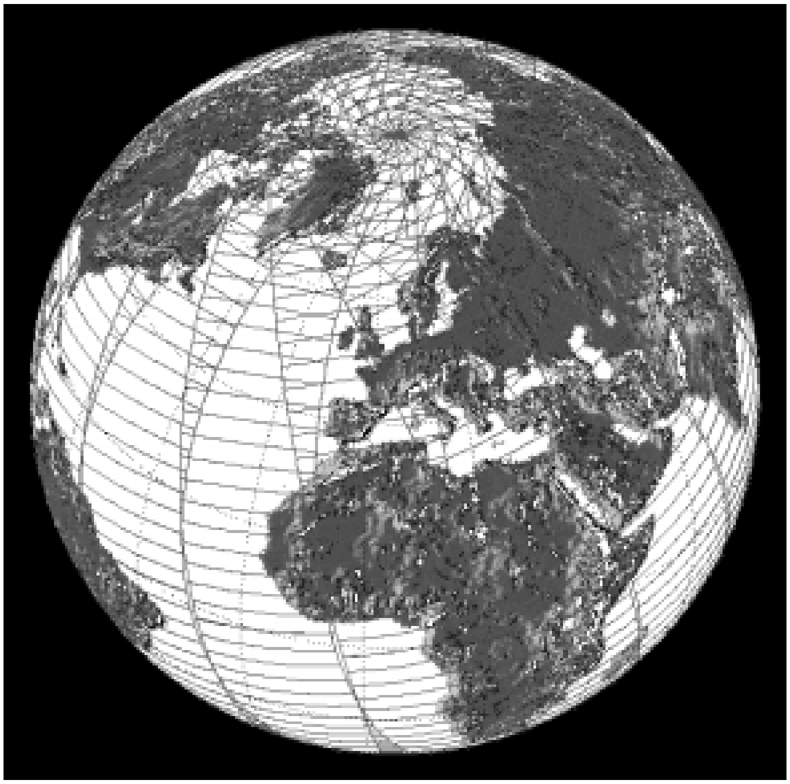


Fig. 2.8. Daily global coverage is achieved in the 2800 km OMI swath in *Global Observation Mode.*

2.2.4.2 OMI Measurement Resolution

The location of ground pixels is accurate to about ±0.1 CCD pixel or 1-2 km, and is determined by a combination of knowledge of spacecraft position and time. In addition, each read-out is accompanied with data (for a single wavelength per CCD detector) for which no co-addition is done. This results in a high spatial sampling (each 2.7 km) in the flight direction. The wavelength is programmable; a possible choice would be 340 nm in the UV and 380 nm in the VIS channel, to enable cloud detection with a high sampling rate.

There are 3 distinct spectral bands: UV-1, UV-2, and visible, which vary in resolution between 0.42 and 0.63 nm. The radiometric accuracy of spectra is best stated as a signal-to-noise ratio, which depends on the signal strength and is relatively poor in the UV, and much better in the visible. Radiometric accuracy of the spectra also depends on stray light and dark current levels.

2.2.5 Coverage Overlap Between Instruments

Fig. 2.9 illustrates the locations for typical atmospheric views from the 4 Aura instruments, during portions of 3 consecutive orbits. The time difference between views from MLS ahead of Aura (about 3000 km away from the satellite) and Aura overpasses at the same locations is about 7 minutes, during which the Earth rotates by ~200 km near the equator (less at higher latitudes). This explains the across-track separation between MLS profiles, spaced by ~165 km along-track, and TES nadir views, spaced by ~550 km along-track, which are also shifted to the “East” (across-track) from the TES limb views as well as the HIRDLS profile locations (“behind” Aura); these shifts will be less at higher latitudes. The symbol sizes (circles for HIRDLS, and “error bars” for MLS and TES limb views) crudely represent the averaging region, although the TES nadir views (dots) are drawn much larger than the actual (scaled) TES nadir footprints (8 km along-track, narrower than the OMI swath, and 5 km across-track). The OMI swaths are centered on the TES nadir views and extend across-track to fill-in between orbits, albeit not completely at the lowest latitudes (which is why a small gap between orbits is shown). HIRDLS profile locations (6 scans/sequence) are shown spaced by ~500 km across-track; this illustrates the desired orbital overlap (for attitude consistency checks), although details such as profile spacing variation as a function of latitude have not been finalized.

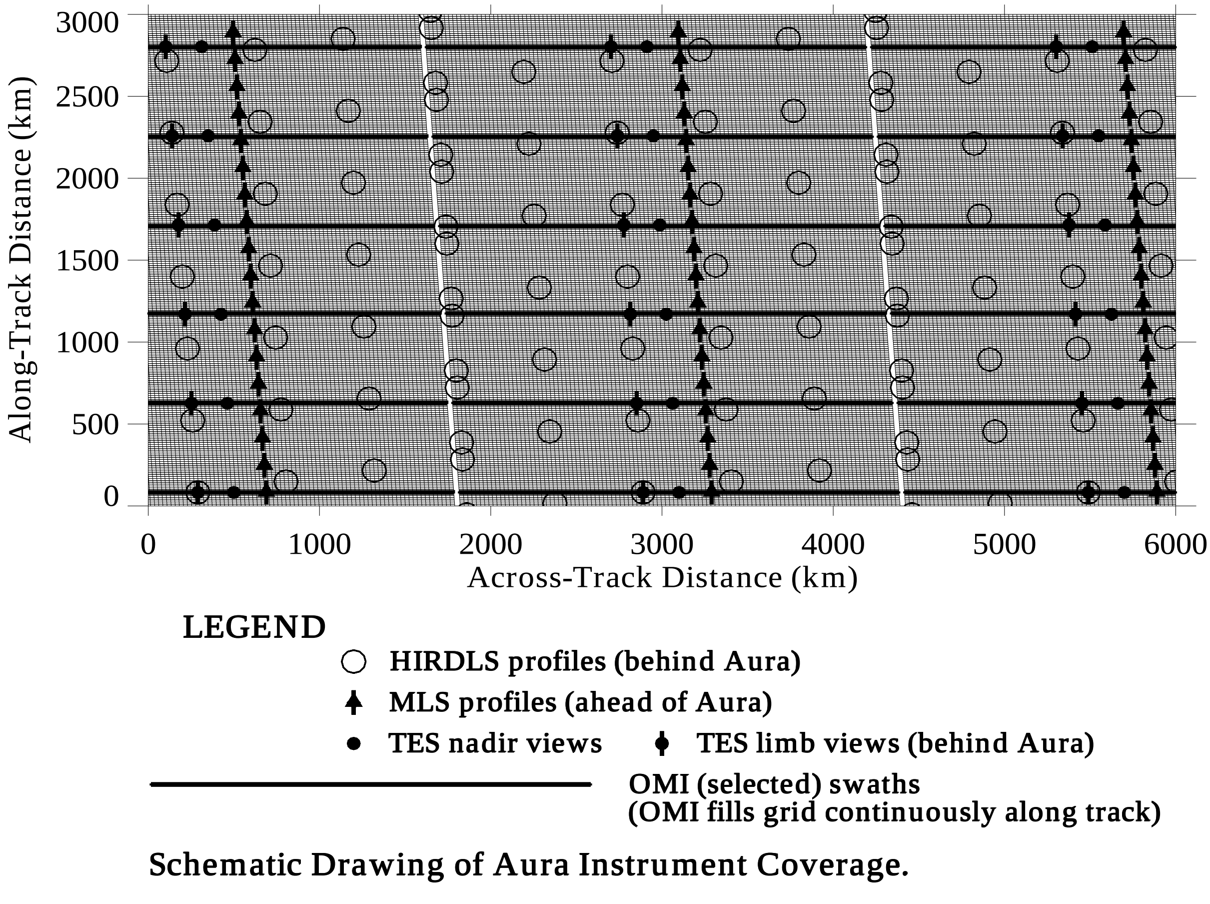


Fig. 2.9. Schematic drawing of measurement coverage and overlap for the four Aura instruments.

3 Aura Science Data Products

A schematic overview of the main atmospheric profiles expected from the Aura suite of measurements is provided in Figure 3.1 below. The majority of the OMI products are column values, as noted in the figure. We describe below the expected Aura products and their vertical range, for each of the four instruments. In each case, a brief sub-section on data processing is included, in order to summarize the plans for processing individual data sets, especially for any aspects that might be relevant for correlative data considerations.

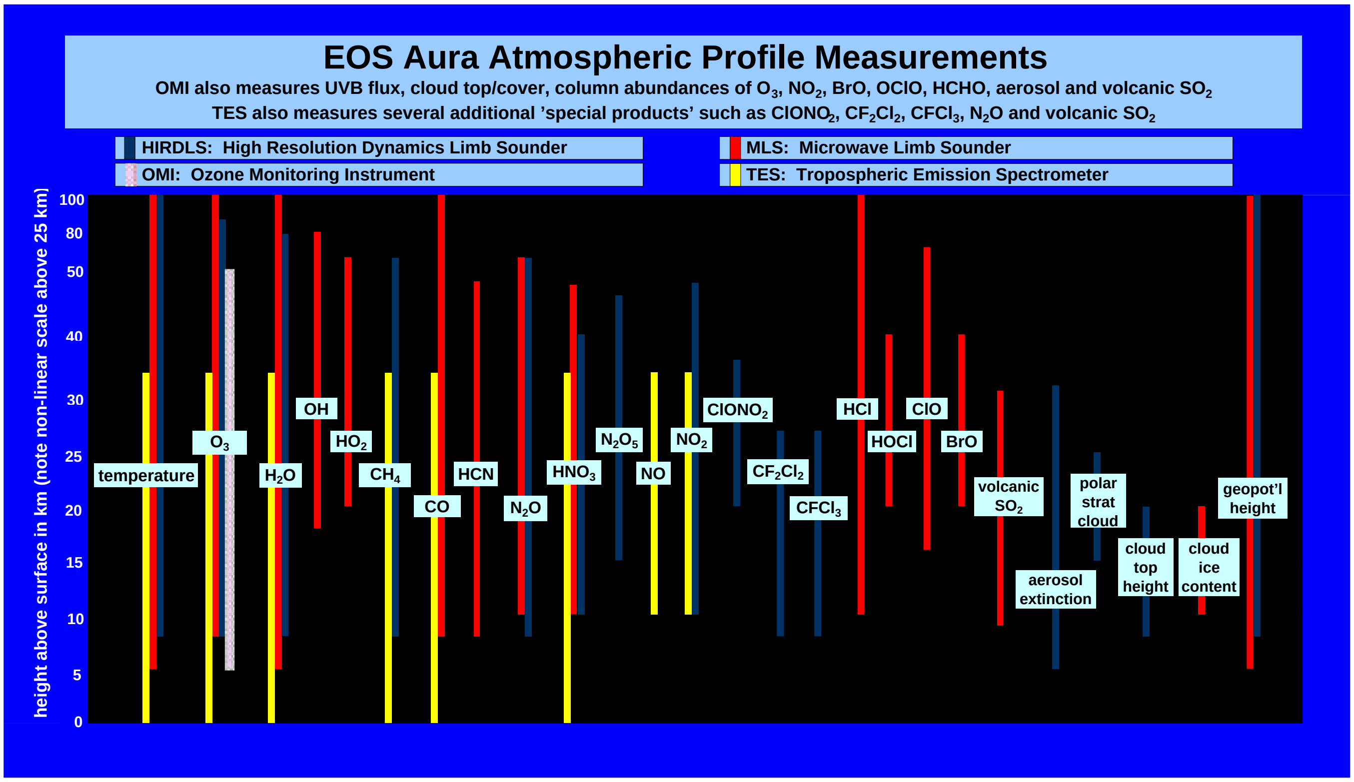


Fig. 3.1. EOS Aura Atmospheric Profile Measurements.

3.1 HIRDLS Science Data Products

3.1.1 HIRDLS Data Processing

The first step in the processing of HIRDLS data is the conversion of raw digital data contained in the instrument telemetry (Level 0 data) into calibrated engineering and science data referred to as Level 1 data. During this initial process, valid atmospheric, space and in-flight calibrator views within the data stream are identified and an attempt is made to identify and flag bad or corrupted data. Line-of-sight pointing direction will be determined from instrument pointing sensor data for each radiance measurement. Associated pointing errors will be estimated. Radiometric conversions will be made based upon pre-launch and in-flight calibration data and measurement noise estimates. These and other required ancillary data will then be written to an HDF-EOS formatted data file for use by the Level-2 processor. Details of the Level-1 data processing algorithm can be found in the HIRDLS Algorithm Theoretical Basis Document, Level 0-1 (SW-HIR-168).

The Level-2 data processing stage ingests Level-1 calibrated radiance and pointing data and generates Level-2 science data products consisting of vertical atmospheric profiles of temperature and the concentration mixing ratios of several trace gases on a fixed pressure grid. In a Level-2 pre-processing step the presence of high cloud in the HIRDLS field-of-view will be detected and its cloud-top pressure determined. Retrieved geophysical profiles are geolocated and placed onto a HIRDLS standard pressure grid with uniformly spaced levels in log pressure.

The physical retrieval approach, based upon Rodgers' optimal estimation approach [Rodgers, 1976, 1990, 2000], will be used to retrieve atmospheric quantities from measured limb radiances. The approach seeks to obtain atmospheric temperature and constituent profiles which produce simulated limb radiances consistent with measured radiance and a priori information. Horizontal gradients in temperature and constituent amounts will be estimated in a two step process. An initial retrieval pass will be made neglecting gradients. These data will be used to produce a 3-D map whereby gradients along the line-of-sight path will be estimated and accounted for in the forward radiance model during a second pass of the retrieval process. Details of the retrieval scheme are given in the HIRDLS Level 2 Algorithm Theoretical Basis Document (SW-HIR-339).

3.1.2 HIRDLS Products

Table 3.1 lists the main products measured by HIRDLS (along with temperature and geopotential height), and their associated height ranges.

Table 3.1. Constituents Measured by HIRDLS.

Formula	Name	titude Range (km)
O_3	Ozone	8–80
H_2O	Water vapor	8–65
CH_4	Methane	8–60
N_2O	Nitrous oxide	8–30
HNO_3	Nitric acid	10–40
NO_2	Nitrogen dioxide	10–55
N_2O_5	Nitrogen pentoxide	15–45
$CFCl_3$	CFC 11	8–30
CF_2Cl_2	CFC 12	8–30
$ClONO_2$	Chlorine nitrate	20–40
Aerosol	Aerosol extinction	8-22, or above

The HIRDLS Level 2 science data product is a daily file, in an HDF-EOS swath format, containing atmospheric profiles of geophysical quantities, such as temperature and constituent mixing ratios, and associated ancillary information, such as profile geographic location, spacecraft location and scan mode information. Table 3.2 below gives a representation of the parameter type, name, a brief description and units. The first eleven parameters are ancillary data used to locate each profile and provide additional information about modes of the instrument and location of the spacecraft. The remaining parameters contain retrieved vertical profiles, where each level in the profile is related to pressure (hPa) by $P(i) = 1000.0 * 10^{(-i/24)}$, for i = 0, 144 (four times the vertical resolution of the UARS pressure surfaces).

Table 3.2. HIRDLS Level 2 Data Product File Description.

Record Detail, Name: HIRDLS2 Frequency:Daily, Record:atmospheric profile, number of records: ~7500

Parameter	**Units**	**Type**	**#/Rec**	**Description**
Time	TAI93	Double	1	TAI93 time for channel 14 50 mb tangent point
Latitude	Degrees	Float	1	Latitude for channel 14 50 mb tangent point
Longitude	Degrees	Float	1	Longitude for channel 14 50 mb tangent point
Orbitdir		Byte	1	Orbit direction: ascending/descending
Scanmode		Short	1	HIRDLS Science Scan Mode
Scandir		Byte	1	Scan Direction: up/down
Solar zenith angle	Degrees	Float	1	Solar Zenith Angle for channel 14 50 mb tang. point
Local Solar time		Float	1	Local Solar Time for channel 14 50 mb tang. point
Spacecraft Latitude	Degrees	Float	1	Spacecraft Latitude for channel 14 50 mb tg. point
Spacecraft Longitude	Degrees East	Float	1	Spacecraft Longitude for channel 14 50 mb tg. pt.
Spacecraft Altitude	km	Float	1	Spacecraft Altitude for channel 14 50 mb tang. pt.
Z	km	Float	145	Profile of Altitudes at each respective pressure level
Temperature	K	Float	145	Profile of Temperature
O3	ppv	Float	145	Profile of Ozone Mixing Ratio
H2O	ppv	Float	145	Profile of Water Vapor Mixing Ratio
ClONO2	ppv	Float	145	Profile of Chlorine Nitrate Mixing Ratio
N2O5	ppv	Float	145	Profile of Nitrogen Pentoxide Mixing Ratio
N2O	ppv	Float	145	Profile of Nitrous Oxide Mixing Ratio
NO2	ppv	Float	145	Profile of Nitrogen Dioxide Mixing Ratio
CH4	Ppv	Float	145	Profile of Methane Mixing Ratio
HNO3	Ppv	Float	145	Profile of Nitric Acid Mixing Ratio
CFC11	Ppv	Float	145	Profile of CFC 11 Mixing Ratio
CFC12	Ppv	Float	145	Profile of CFC 12 Mixing Ratio
Aerosol01	1/km	Float	145	Profile of Aerosol Extinction from Channel 1
Aerosol06	1/km	Float	145	Profile of Aerosol Extinction from Channel 6
Aerosol13	1/km	Float	145	Profile of Aerosol Extinction from Channel 13
Aerosol19	1/km	Float	145	Profile of Aerosol Extinction from Channel 19
Temp. Precision	K	Float	145	Profile of Temperature Precision
Pressure Precision	Hpa	Float	145	Profile of Pressure Precision
O3 Precision	Ppv	Float	145	Profile of Ozone Mixing Ratio Precision
H2O Precision	Ppv	Float	145	Profile of Water Vapor Mixing Ratio Precision
ClONO2 Precision	Ppv	Float	145	Profile of Chlorine Nitrate Mixing Ratio Precision
N2O5 Precision	Ppv	Float	145	Profile of Nitrogen Pentoxide Mixing Ratio Precis.
N2O Precision	Ppv	Float	145	Profile of Nitrous Oxide Mixing Ratio Precision
NO2 Precision	Ppv	Float	145	Profile of Nitrogen Dioxide Mixing Ratio Precision
CH4 Precision	Ppv	Float	145	Profile of Methane Mixing Ratio Precision
HNO3 Precision	Ppv	Float	145	Profile of Nitric Acid Mixing Ratio Precision
CFC11 Precision	Ppv	Float	145	Profile of CFC 11 Mixing Ratio Precision
CFC12 Precision	Ppv	Float	145	Profile of CFC 12 Mixing Ratio Precision
Aerosol01 Precision	1/km	Float	145	Profile of Aerosol Extinction Precision
Aerosol06 Precision	1/km	Float	145	Profile of Aerosol Extinction Precision
Aerosol13 Precision	1/km	Float	145	Profile of Aerosol Extinction Precision
Aerosol19 Precision	1/km	Float	145	Profile of Aerosol Extinction Precision

Record Detail, Name:HIR2CLD, Frequency:Daily,Record:Single Point,Number of Records:~22500				
Parameter	**Units**	**Type**	**#/Rec**	**Description**
Time	TAI93	Double	1	TAI93 time for channel 14 50 mb tangent point
Latitude	Degrees	Float	1	Latitude for channel 14 50 mb tangent point
Longitude	Degrees	Float	1	Longitude for channel 14 50 mb tangent point
Orbitdir		Byte	1	Orbit direction: ascending/descending
Scanmode		Short	1	HIRDLS Science Scan Mode
Scandir		Byte	1	Scan Direction: up/down
Solar zenith angle	Degrees	Float	1	Solar Zenith Angle for channel 14 50 mb tangent point
Local Solar time		Float	1	Local Solar Time for channel 14 50 mb tangent point
Spacecraft Latitude	Degrees	Float	1	Spacecraft Latitude for channel 14 50 mb tangent point
Spacecraft Longitude	Degrees East	Float	1	Spacecraft Longitude for channel 14 50 mb tang. point
Spacecraft Altitude	km	Float	1	Spacecraft Altitude for channel 14 50 mb tangent point
Cloud Top Pressure	hPa	Float	1	Pressure of cloud top for this detector column
Column Number		Short	1	Detector column number (1,2,3)

All ancillary data are reported with every HIRDLS profile, including time, tangent point information, scan mode and direction, and spacecraft location. The time is reported in International Time (TAI93) at the 50 hPa pressure level. The tangent point information includes: latitude, longitude, local time and solar zenith angle, for the 50 hPa level. Spacecraft location is reported in ECR coordinates respective to the 50 hPa level.

The HIRDLS Level 2 standard data products will adhere to the Aura Standard Data Format Guidelines Paper, which was adopted by the Aura Data Systems Working Group and is available at: http://www.eos.ucar.edu/hirdls/HDFEOS_Aura_File_Format_Guidelines.pdf.

3.1.3 HIRDLS Product Uncertainties

We list in Table 3.3 the required precision and accuracy of HIRDLS geophysical measurements.

Table 3.3. HIRDLS requirements for precision and accuracy.

Parameter	Precision	Absolute Accuracy
Temperature	0.4 K below 50 km 1 K above 50 km	1 K below 50 km 2 K above 50 km
Constituents	1–5%	5–10%
Aerosol extinction	1-5%	5-25%
Height gradient	20 m / 500 km	N/A

3.2 MLS Science Data Products

3.2.1 MLS Data Processing

Data processing for EOS MLS follows the standard EOS processing Levels, namely processing from Level 0 data (raw counts, voltages) to Level 1 data (calibrated radiances and their uncertainties), Level 1 to Level 2 (retrieved geophysical products and their uncertainties), and Level 2 to Level 3 (derived products such as mapped fields or zonal mean values). Algorithm details can be found in the EOS MLS "ATBDs"; see Jarnot [1999] for Level 1, Livesey and Wu [1999] for Level 2, Read [1999] for the forward model, Jiang [2000] for Level 3 mapping algorithms, and Wu and Jiang [2001] for cloud measurements. All profiles will be retrieved in daily files, following a repeatable coverage (see section 2.2.2.2), barring any power sharing mode need, occasional calibration periods, or other unexpected events. The nominal Level 3 grid is chosen with grid centers at -81, -79, -77, ..., -3, -1, 1, 3,...77, 79, 81 degrees of latitude, and at 2, 6, 10, ... 358 degrees longitude. The gridded products (such as daily maps) will nominally be produced on a monthly basis (using Salby's Fourier methodology); this is also true for the zonal mean products (typically daily and monthly means are to be produced), see Waters [1999] and Jiang [2000] for more details.

3.2.2 MLS Products

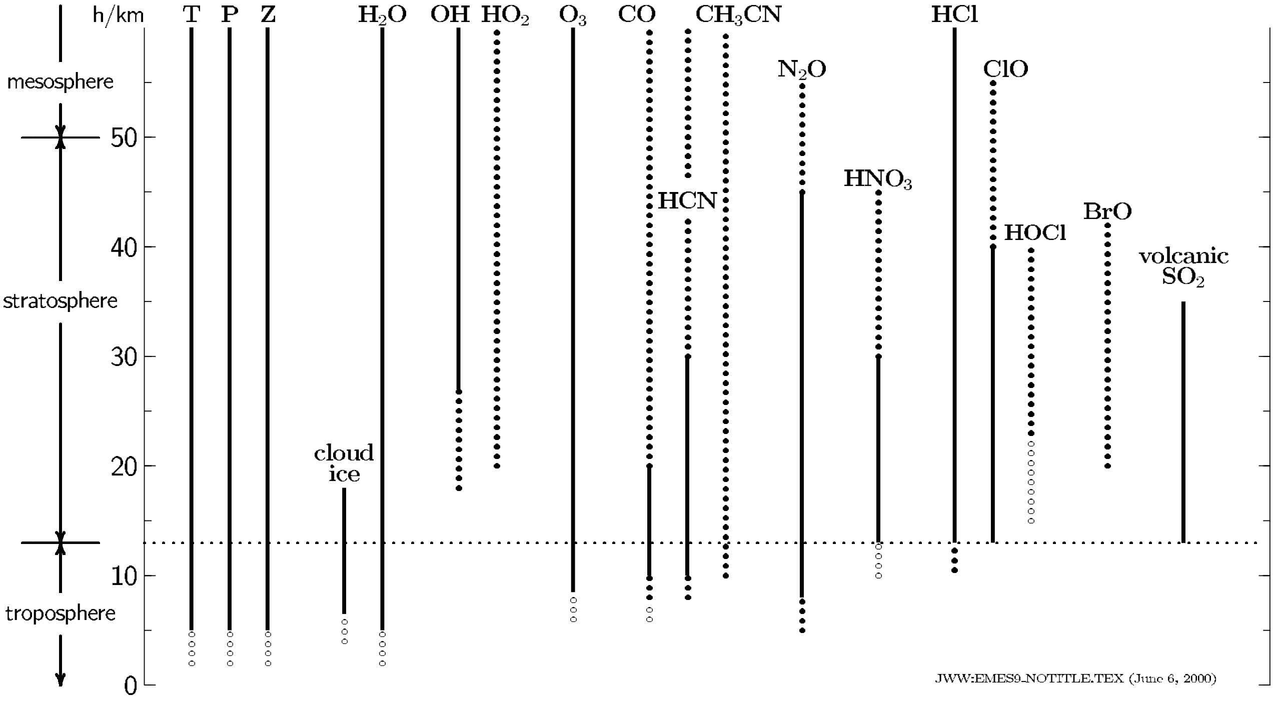


Figure 3.2. EOS MLS scientific data products. T is temperature, P is pressure, and Z is geopotential height. Solid lines indicate useful individual profiles and/or daily maps. Dotted lines indicate that zonal (or other) averages will likely be needed to obtain useful precision. Open circles indicate goals for more difficult measurements. Measurements of T, P, Z, H_2O, O_3, HCl, OH and CO extend higher than the 60 km indicated here. It should be noted that 'useful profiles' indicated by the solid lines here do not necessarily apply at all times of day and night due to diurnal variation in species such as OH, HO_2, ClO and BrO. Also, they do not necessarily apply at all latitudes due to latitudinal variation in abundances. For example, although useful individual profiles of lower stratospheric HNO_3 will be obtained at mid and high latitudes, they are not expected in the tropics because of the smaller HNO_3 abundances at low latitudes.

The MLS science data products are summarized in Fig. 3.2 above. The definition for most of these is straightforward, but cloud products deserve a somewhat more detailed description. A separate theoretical basis document (Wu and Jiang, 2001) describes the plans for extracting cloud products from the MLS measurements. In brief, cloud extinction coefficients (km^{-1}) along the line of sight will be retrieved at the 4 main radiometer (GHz) frequencies, for altitudes between about 5 and 20 km. Ice water content (g/m^3) is another cloud product to be retrieved, although not as part of the first production processing, since this is considered to be a research product.

The MLS measurements come from five different radiometers. Figure 3.3 gives added information about the source of information from each radiometer. Since several products are retrieved from more than one spectral region and radiometer, this information will be used as a consistency check, based on diagnostic products with separate retrievals from different regions. When appropriate, an optimum estimate combining all spectral data in an optimum retrieval will be used as the final product for scientific studies.

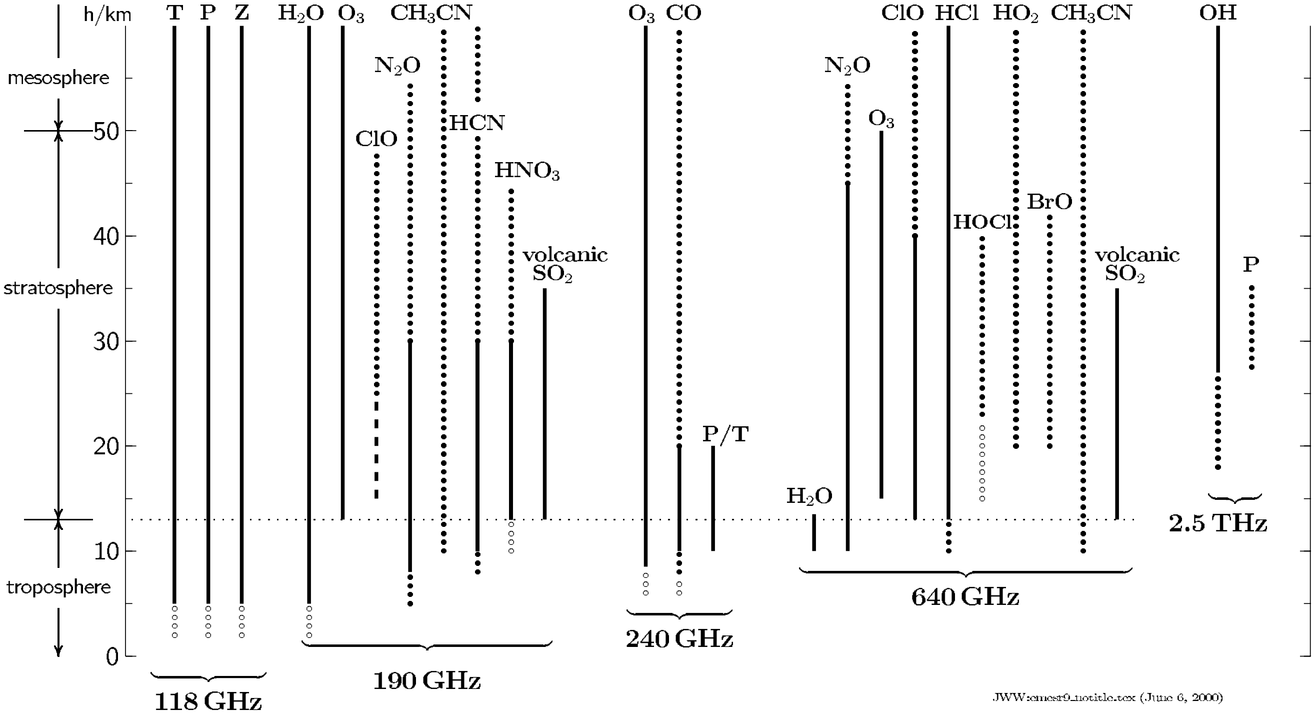


Figure 3.3. Geophysical measurements by individual MLS radiometers. Solid lines indicate useful individual profiles and/or daily maps, dotted lines indicate zonal (or other) averages, the dashed line indicates enhanced ClO in the polar winter vortices. Open circles are goals for more difficult measurements. Measurements of T, P, Z, H_2O, O_3, HCl, OH and CO extend higher than the 60 km indicated here. The cirrus ice measurement, not shown here, is obtained from a combination of observations from the 118, 190, 240 and 640 GHz radiometers. The signal from the spacecraft gyroscope is used with 118 GHz pressure (P) measurements to provide geopotential height Z. The 2.5 THz measurement of P provides information on the offset between the pointing references for the THz and GHz fields-of-view.

3.2.3 MLS Product Uncertainties

MLS Precision

Table 3.4 gives the list of geophysical products for EOS MLS, along with the expected single-profile precision values at various altitudes. For products with poor single-profile precision (e.g., BrO, HOCl, HO_2, and lower stratospheric OH, as listed in Table 3.4), Level 3 zonal mean data products will be a more useful scientific product [see Waters, 1999].

Table 3.4. Expected precision (1σ) for MLS products, based on Filipiak [1999]. Values are for ~ 3 km vertical resolution (retrieval grid). Precision plots for all altitudes, and for different latitudes and vertical resolutions, along with comments on the potential impact of thick clouds, can be found in the above reference; see also Waters [1999].

Geophysical Parameter	**Approximate Vertical Range Of Usefulness**	**Precision for Level 2 Single profiles**[1]	**Precision for Profile averages (monthly 5° zonal means)**
Temperature	5 – 80 km	~ 2 K @ 40 km ~ 1 K @ 5 – 30 km	
Geopotential height	5 – 80 km	~ 60 m @ 50 km ~ 20 m @ 5 – 40 km	
BrO	20 – 40 km		~ 6 pptv @ 40 km ~ 2 pptv @ 20 km
CH_3CN	10 – 50 km	~ 50 pptv @ 15-40 km	~ 2 pptv @ 15-40km
ClO	15 – 50 km	~ 0.6 ppbv @ 40 km ~ 0.2 ppbv @ 20 km	
CO	10 – 80 km	~ 50 ppbv @ 10 – 25 km	
HCl	15 – 80 km	~ 1 ppbv @ 50 km ~ 0.3 ppbv @ 15 – 30 km	
HCN	10 – 50 km	~ 0.1 ppbv @ 10 – 30 km	
HNO_3	15 – 40 km	~ 3 ppbv @ 15 – 25 km	
HOCl	20 – 40 km		~ 40 pptv @ 40 km ~ 10 pptv @ 20 km
HO_2	25 – 50 km		~ 100 pptv @ 50 km ~ 10 pptv @ 25 km
H_2O	5 – 80 km	~ 20% @ 50 km ~ 10% @ 35 km ~ 5% from 5 km to tropopause	
N_2O	10 – 50 km	~ 50 ppbv @ 40 km ~ 20 ppbv @ 20 km	
OH (“upper” strat. and mesosphere)	25 – 80 km	~ 0.1 ppbv @ 50 km ~ 0.01 ppbv @ 30 km	
OH (lower strat.)	18 – 25 km		~ 0.3 pptv
O_3	10 – 80 km	~ 10% @ 50 km ~ 2% @ 30 km ~ 10% within 3 km above trop. ~ 10 ppbv within 3 km below tropopause (in the tropics)	
SO_2 (volcanic)	15 – 35 km	~ 2 ppbv @ 15 – 35 km	
Cloud ice	10 – 20 km	~0.001 gm/m^3 avg. over MLS FOV within ~ 5 km of tropical tropopause ~ 0.005 gm/m^3 avg. over MLS FOV within ~ 2 km of high lat. tropopause	

[1] MLS L2 profiles are produced every 165 km along the measurement track (see Figure 2.2).

There are limitations to Table 3.4 for percent precision values, since these values apply for certain atmospheric conditions and could differ significantly under dissimilar atmospheric conditions. More complete information can be found in the MLS document by Filipiak [1999], giving precision estimates for low and high latitude conditions, where the atmospheric profiles can differ significantly, depending on the parameter. Refined values will be produced by future versions of the MLS retrieval software, through simulated retrievals of increasingly realistic instrument and atmospheric parameters [see Livesey and Wu, 1999].

MLS Accuracy

The first-order understanding of expected accuracies for EOS MLS geophysical products is based on similarities with UARS MLS. Expected values for MLS product accuracy, defined here as the average systematic component of the uncertainty, are tabulated in the 1999 EOS Reference Handbook. The expectations for accuracy values are in the 3 to 10 % range for most products and heights. The final retrieval, the forward model, final instrument and spectroscopic parameters, and an assessment of post-launch error sources contribute to accuracy estimates, thus definitive accuracy estimates will not be available until after launch.

3.3 TES Science Data Products

3.3.1 TES Data Processing

TES data processing falls into 3 groups:

(1) At Level 1A, the raw data from the spacecraft are decommutated and the instrument outputs (called *interferograms*) reconstructed. File headers contain important ancillary data such as time, date, spacecraft and target location, and instrument pointing angle.

(2) At Level 1B, the interferograms are converted to spectra, radiometrically-calibrated and resampled onto a common frequency grid. Certain data quality flags are added to the header at this juncture and the results passed to Level 2.

(3) At Level 2, vertical concentration profiles of the selected species are extracted from the data through a process of *retrieval*; these are essentially simultaneous for all species.

Briefly, all modern retrieval algorithms are somewhat alike. The appropriate version of the Equation of Radiative Transfer is solved to provide an estimate of the expected spectral radiance as seen by the instrument based on an initial estimate of the physical/chemical state of the atmosphere at the time and location of the observation (the so-called *first guess*). This *forward model* is compared to the true spectral radiance and the parameters of the atmospheric state are adjusted (using specified rules) to bring the forward model into closer agreement with the observation. The process is iterated until, by other specified rules, convergence is achieved. The resulting *state vector* of atmospheric parameters is the desired result. Most algorithms, including the one described here, also provide an objective estimate of the accuracy of the retrieval.

3.3.2 TES Products

The TES standard data products are listed in Table 3.5. Standard product species profiles are reported at the standard pressure levels listed in Table 3.6. For each species at each level the following five parameters are reported:

(1) volume mixing ratio (VMR) with respect to dry air;

(2) random error estimate (i.e. the square root of the diagonal elements of the output covariance matrix);

(3) systematic error estimate;

(4) fraction of explained variance, which gives the relative contribution of the data and the a priori to the reported VMR;

(5) correlation length, which is a measure of the independence of adjacent and nearby levels.

Table 3.5. TES Standard Products.

	Product	Nadir	Limb
1	Level 1A Interferograms	√	√
2	Level 1B Spectroradiances	√	√
3	Atmospheric Temperature Profiles	√	√
4	Surface Temperature	√	
5	Land Surface Emissivity	√	
6	Ozone (O_3) VMR Profile	√	√
7	Water Vapor (H_2O) Profile	√	√
8	Carbon Monoxide (CO) VMR Profile	√	√
9	Methane (CH_4) VMR Profile	√	√
10	Nitric Oxide (NO) VMR Profile		√
11	Nitrogen Dioxide (NO_2) Profiles		√
12	Nitric Acid (HNO_3) VMR Profile		√

Table 3.6. TES standard product reporting pressure levels.

Index	Pressure	US Standard Atmosphere Altitude[1]	Delta Altitude
	HPa	km	km
0	1000.0	0.100	
1	681.3	3.175	3.075
2	464.2	6.100	2.925
3	316.2	8.825	2.725
4	215.4	11.350	2.525
5	146.8	13.800	2.450
6	100.0	16.200	2.400
7	68.1	18.650	2.450
8	46.4	21.100	2.450
9	31.6	23.600	2.500
10	21.5	26.100	2.500
11	14.7	28.600	2.500
12	10.0	31.200	2.600
13	6.8	33.800	2.600
14	4.6	36.600	2.800

[1] Actual altitude will depend on the temperature profiles.
The altitudes and delta altitudes listed in the Table are only a coarse guide.

Because TES observes over broad regions of the infrared spectrum, a large suite of atmospheric species will be retrievable from the TES spectro-radiances. A partial list of these, designated as special products, is given in Table 3.7.

Table 3.7. TES Special Products (Partial List).

H_XO_Y	C-compounds	N-Compounds	Halogen-Compounds	S-Compounds
H_2O_2	C_2H_6	HO_2NO_2	HCl^*	SO_2
HDO	C_2H_2	NH_3	$ClONO_2$	COS
	HCOOH	HCN	CCl_4	H_2S^*
	CH_3OH	N_2O^{**}	CCl_3F	SF_6
	PAN	N_2O_5	CCl_2F_2	
	$CH_3C(O)CH_3$		$CHCl_2F$	
	C_2H_4		$CHClF_2$	

*Volcanic plume column densities only **Tropospheric Control (VMR known)

3.3.3 TES Product Uncertainties

Many factors, ranging from instrumental effects to details of retrieval algorithm to line-parameter errors, contribute to errors in the retrieved products. In addition, there is often a trade-off between vertical and spatial resolution, and precision. While many of the details required to make accurate estimates of the uncertainties remain to be determined, the TES system (instrument and data retrieval process) is designed to provide temperature profiles with errors of less than 1 K and species profiles with errors of less than 10%. In many circumstances, accuracies may be substantially better.

3.4 OMI Science Data Products

3.4.1 OMI Data Processing

Data processing for EOS OMI, with the exception of near real time (NRT) and very fast delivery (VFD) products, will follow the standard EOS processing levels. Level 0 data will be processed to Level 1B data (calibrated radiances and irradiances and their uncertainties, geolocation data and metadata); Level 1B and other data to Level 2 data (retrieved geophysical products and their uncertainties, geolocation data and metadata). All Level 2 data will have daily global coverage. The NRT and VFD products will not be processed following the standard EOS procedures; NRT products (ozone column density and ozone profile) will be processed from “rate buffered data” (intermediate level between 0 and 1B) and made available within 3 hours of the observation, with global daily coverage. VFD products are experimental. They are retrieved from Level 0 data measured during part of the orbit, to be downloaded once a day over Finland and processed at FMI. The VFD products – ozone column density, ozone profile, HCHO column density, UV-B flux and UV spectra – will have limited geographical coverage (2600 km swath from the Arctic ocean to the Alps) and will be delivered on a daily basis.

3.4.2 OMI Products

The OMI Level 1B products that must be validated are spectral solar irradiance, and spectral Earth radiance. The OMI Level 2 (and Level 1B) products and expected accuracies are described in Table 3.8 below. The definition of most products is straightforward, but OMI aerosol optical thickness, cloud scattering pressure, and cloud fraction need to be described in more detail.

The spectral aerosol optical thickness (AOT) is the aerosol extinction integrated over a vertical path from the ground to outer space. The retrieval algorithm uses approximately

18 narrow wavelength bands between 340 and 500 nm and applies to cloud-free regions only. For these regions, the measured reflectances are compared to computed reflectances for different aerosol types from a radiative transfer model. The spectral variation of the aerosol optical thickness, commonly expressed as the Ångstrom coefficient, is a measure for the aerosol size distribution.

The cloud fraction *c* of a ground pixel is derived from the contrast between the surface and a cloud. The algorithm yields an effective cloud fraction, because an optically thick cloud is assumed. Besides the cloud cover, it is also important to get information about the pixel homogeneity.

The cloud pressure will be determined in two ways: from the Ring effect in the Fraunhofer Ca II lines around 394 nm, as has been done for SBUV [Joiner and Bhartia, 1995; Joiner et al., 1995], and by applying the DOAS (Differential Optical Absorption Spectroscopy) method. The DOAS method will be applied using the absorption features of the O_2-O_2 collision complex near 477 nm. It is expected that the two methods will be complementary and that combining these two methods may result in a more accurately determined cloud pressure.

3.4.3 OMI Product Uncertainties

See Table 3.8 for a listing of expected accuracies. The accuracy is defined here as the combination of all random and systematic errors with *known* magnitude. The reason for this is that it should be possible to test whether the requirements given here will be met. The pragmatic definition of the accuracy therefore is: the rms difference between 1) product values retrieved from simulated (“measured” and calibrated) theoretical Earth radiance spectra generated with a state of the art radiative transfer model (including well-defined atmospheres) and 2) the input product values used for the generation of these spectra. The theoretical spectra should be fed into instrument simulation software (“measured”), with all known error sources included; and calibrated with level 0-1B available directly after launch software. Hence the accuracy is determined by systematic and random errors in the retrieval and calibration algorithms, and by systematic and random errors associated with the measurement technique. Note that this definition of accuracy is different from the usual definition (i.e. the average difference between the retrieved value and the “true” value). Many known systematic and random error sources with unknown magnitude, such as interference due to partially cloudy scenes, are not included in the present definition of the accuracy.

Table 3.8 Overview of the Level 1B product requirements for the priority ‘A’ and ‘B’ OMI data products.

Data product	**Spectral Range [nm]**	**Ground pixel size [km × km]**	**Spectral knowledge [CCD pixel]**	**Radiometric accuracy[1] [%]**	**Radiometric precision[2] [S/N]**
Ozone column ● *DOAS* ● *TOMS*	 320 – 340 310 – 380	 20 × 20 20 × 20	 0.01 0.33	 ≤ 3 ≤ 1	 ≥ 250 ≥ 300
Ozone profile	270 – 340	40 × 40	0.02	≤ 1	λ < 310 ≥ 100
Aerosol optical thickness	340 – 500	20 × 20	not critical	≤ 1	≥ 500
Aerosol single scattering albedo	340 – 500	20 × 20	not critical	≤ 1	≥ 500
NO$_2$ column	425 – 450	40 × 40	0.02	≤ 3	≥ 5800
Cloud scattering pressure	390 – 400 470 – 485	20 × 20 20 × 20	0.01 0.01	≤ 3 ≤ 3	not critical ≥ 1600[3]
Cloud fraction	320 – 500	20 × 20	not critical	≤ 1	not critical
Surface UV-B	280 – 400	20 × 20	not critical	not critical	not critical
SO$_2$ column	300 – 330	40 × 40	0.01	≤ 3	≥ 400
BrO column	344 – 360	40 × 40	0.02	≤ 3	≥ 2500
OClO column	355 – 385	40 × 40	0.01	≤ 3	≥ 1500
HCHO column	335 – 360	40 × 40	0.01	≤ 3	≥ 3200
Surface reflectance	320 – 500	20 × 20	not critical	≤ 1	≥ 100
UV spectra	280 – 400	20 × 20	not critical	not critical	not critical
Near Real Time Products					
Ozone column	320 – 340	20 × 20	0.02	≤ 3	≥ 100
Ozone profile	270 – 340	40 × 40	0.02	≤ 1	λ < 310 ≥ 100
Very Fast Delivery Products					
Ozone column Surface UV-B flux	320 – 340 280 – 400	20 × 20 20 × 20	0.02 not critical	≤ 3 not critical	≥ 100 not critical
Ozone profile	270 – 340	40 × 40	0.02	≤ 1	λ < 310 ≥ 100
UV spectra	280 – 400	20 × 20	not critical	not critical	not critical
HCHO column	335 – 360	40 × 40	0.01	≤ 3	≥ 3200

Note 1) The radiometric accuracy defined here refers to the reflectivity (i.e. ratio of the Earth radiance and the solar irradiance)
Note 2) S/N requirements are valid for the given ground pixels size in column 3 (i.e. the same ground pixel sizes as in Table 3.1)
Note 3) The most stringent requirement on radiometric precision is given by the method using the 477 nm O$_2$-O$_2$ collision complex.
Note 4) A requirement noted as not critical means that other products demand stronger requirements for the Level 1B product.

4 Aura Plans for Pre-launch Activities Relating to Validation

We summarize here the plans for a number of pre-launch activities relating to validation, since successful validation is a process and cannot occur without certain critical steps. These include careful instrument calibration (see section 4.1 for a brief reference/summary), and algorithm development for the retrieval of geophysical data products, with simulations and algorithm testing (or algorithm "pre-launch validation", see section 4.2). In addition to these topics, we describe in section 4.3 the Aura needs and priorities for spectroscopic data and other databases. Later improvements in such databases could improve the accuracy of Aura reprocessed data.

4.1 Instrument Calibration

4.1.1 HIRDLS Calibration

The accuracy and precision of retrieved science data depends critically on knowledge of the instrument response to incident radiation. It is the purpose of pre-launch instrument testing and calibration to quantify the response of the instrument over a range of operating conditions to very precise levels. The details of the instrument calibration and testing can be found in the Pre-launch Calibration Plan (TP-HIR-007) and in the HIRDLS Proto-Flight Model Instrument Test Plan (TP-LOC-204). An overview of the calibration and testing plan is presented below.

Instrument level functional and performance testing at the instrument integrator's facility will include tests to verify that the instrument performs to the required levels and that the instrument response is stable and repeatable. Critical among the performance tests will be the calibration of scan mirror encoders over the full range of scan angles. Additionally, the in-flight calibrator and mirror temperature sensors will be characterized and calibrated at the subsystem level.

Formal instrument calibration will be performed at the Oxford University test and calibration facility. The instrument will be in a thermal-vacuum chamber with the instrument surrounded by temperature controlled walls and mounted on an optical table along with radiometric test equipment, and isolated from mechanical vibrations. Testing will be performed under operations conditions that closely simulate the expected on-orbit environment.

The absolute radiometric response to a known laboratory source, varied over a range of source temperatures, will be measured. In addition, the in-flight calibrator will be calibrated against a standard laboratory source. Precise knowledge of the relative spectral response of each of the 21 science channels to the 1% level is necessary for inclusion in the data processing algorithms. Measurements by a vacuum compatible monochromator will be made to the required sensitivity. A lower resolution search for out-of-band spectral leaks of the order of 0.1% of the peak in-band response will be made.

Knowledge of the relative vertical spatial response is necessary for inclusion in the data processing algorithms and therefore the spatial response of each of the 21 spectral channels will be measured using a narrow slit with an accuracy of ± 0.5% of the peak response and with adequate angular resolution to resolve small-scale variations in the response. The relative positions of the detector fields-of-view will be mapped. Any unexpected response to radiation occurring at off-axis angles will be characterized.

4.1.2 MLS Calibration

Calibration of the MLS instrument involves four major categories, similar to the case of the UARS MLS instrument: 'radiometric calibration,' giving the (frequency-dependent) transformation from power incident upon the antenna to output radiance units, 'field-of-view (FOV) calibration,' giving the response of the instrument to the input signal as a function of the angle at which the signal is incident upon the antenna, 'spectral calibration,' giving the relative response of the instrument to the input signal within each frequency channel (including the response in primary and image sidebands), and 'engineering calibration,' giving the output of engineering sensors. The plans for calibration of EOS MLS are described by Jarnot [1999]; see also the overview document by Waters [1999]. The instrument calibration leads to certain important instrument parameters, to be used by the forward model for simulating the expected radiances. A description of the forward model for EOS MLS is given by Read [1999].

4.1.3 TES Calibration

There are many elements of the TES instrument that are calibrated either at the subassembly level or after the instrument is fully integrated (see also the TES Instrument Calibration Plan). While the calibration of all these elements, many of them engineering measurements, is important to the TES mission, four are essential for the accurate conversion from data numbers to a retrieved geophysical parameter. The four are: 1) radiometric response, 2) field-of-view response, 3) detector co-alignment and 4) instrument (spectral) line-shape.

Radiometric Response

The radiometric response of the instrument is required to convert from data numbers (DN) to radiances. In TES, as with all instruments operating in the mid-infrared, this conversion will change with time and requires near continuous radiometric calibration measurements to assure accurate radiances. To achieve the required accuracies TES carries onboard a radiometric calibration source. The source is a high emissivity, cavity blackbody whose radiometric output is calibrated to better than ± 0.1 K in brightness temperature over the 290K - 340K range. It is designed to maintain this accuracy throughout the 5-year life of the Aura mission. In flight this source is viewed once every ~80 s. Observations of the blackbody are combined with measurements of cold space, also made every 80 s, to provide near continuous updates to the linear radiometric calibration coefficients. Pre-flight calibration of the radiometric source is carried out at three levels. At the subsystem level (i.e., the source only and its associated electronics) the spectrally resolved source radiance is compared to a standard radiometric source. At the instrument level, spectrally resolved radiances of the radiometric source and of an external high-accuracy radiometric source are measured and compared in the flight configuration. Finally, the radiometric output of the external calibration source is measured with a NIST standard infrared radiometer.

Field-of-view response

The TES detectors view over a volume of the atmosphere. At the limb where vertically resolved radiances are required, knowledge of the response-weighted area of the projected volume is essential for accurate modeling of the measured radiances in the retrieval of geophysical parameters. The field-of-view response depends on the design and alignment of the instrument optics, the area of the detector elements, and on the spatial response of the detectors. The instrument is designed so that these parameters will remain constant over the duration of the mission. Pre-flight characterization of the field-of-view response is carried out with the instrument in its flight-configuration. The field-of-view response is measured by scanning a small, well-defined line or spot source, optically located at infinity, across the field-of-view of the instrument while recording the detector signals. The measurements, after appropriate analysis and interpolation, are used directly in the retrieval algorithm. This measurement will also detect any significant near-field stray light response and will determine relative alignment between the detector arrays.

Detector array co-alignment

TES uses four detector arrays each observing in a different wavelength range. Absolute knowledge of limb view tangent height is required for each array. For the 2B array (see section 2.2.3), this knowledge is determined by the retrieval of atmospheric pressure. Knowledge for the other three arrays is determined from measurements of their relative alignment with respect to the 2B array. On the instrument, the four arrays are mounted in two separate opto-mechanical assemblies, each housing two arrays. The design of the assemblies is such that within an assembly the two arrays will maintain their relative alignment to a high degree of precision and this co-alignment should be adequately characterized by the preflight field-of-view response measurement described above.

Instrument line shape

The TES instrument, like all spectrometers, modifies the natural shapes of spectral lines. In effect, the instrument convolves a function called the instrument line shape (ILS) with the spectrum of incoming radiation. Accurate knowledge of the ILS is required to accurately model the measured radiances in the retrieval. In an interferometer, the primary parameter controlling the ILS is the maximum optical path difference of the recorded interferogram. Other factors influencing the ILS are the optical alignment of the instrument, the position of the detectors with respect to the optical axis and the throughput of the optical system as a function of the optical path difference. Characterization of the ILS is an important pre-flight calibration activity. The characterization measurements involve the acquisition of spectra whose natural line shapes are accurately known. Briefly, spectra of pure gasses contained in a gas cell of known length are acquired during pre-flight thermal vacuum testing. The gasses are chosen so that all instrument spectral ranges have spectral features. Model gas cell spectra are calculated using a standard radiative transfer program and compared to the measured spectra. The instrument contribution to the measured line shape is determined by fitting the measured spectrum with the calculated spectrum convolved with a parameterized ILS function.

4.1.4 OMI Calibration

The calibration issues for OMI are:

1. wavelength assignment
2. radiometric calibration
3. ground pixel location
4. corrections for dark current, straylight, gain, readout and electronic noise, etc.
5. slit functions
6. possibly residual polarization (although this is currently not expected to influence the geophysical data products)

Initial wavelength alignment is obtained on the ground, using various narrow line sources. In-flight calibration is obtained using Fraunhofer lines in the solar spectrum as well as in the Earth’s radiance spectrum.

Similarly, initial radiometric calibration is obtained on the ground, using white light sources. In-flight, the Sun is used as a direct calibration source, since its variation over time in the near-UV and visible is negligible.

Ground pixel location is an issue of internal alignment of the instrument (the two CCDs with respect to the instrument) and the instrument to the spacecraft. Current interface requirements meet the OMI scientific requirement of ±1 km.

Dark current, straylight, gain, and noise are measured carefully pre-flight. In-flight monitoring will be done to follow the character of these features, starting with an extensive, in-flight calibration period.

Slit functions will be measured during on-ground calibration. Stray light will be characterized in both the development and the flight model programs. Results will be used in the Level 0→ 1B processor. Detailed descriptions of the calibration issues can be found in the OMI calibration requirements document (draft, Snel [1999]).

4.2 Algorithm Testing

Algorithm testing is necessary, since the quality of retrieved products is limited by the quality of the algorithms, including the accuracy of the forward model. Post-launch validation efforts are in many ways directed towards validation of the algorithms, whereas the algorithm tests before launch can provide a pre-launch validation (assuming "ideal" conditions). Simulated retrievals provide an obvious means to test the quality of the retrievals, although this is typically tested under optimum conditions of a "perfect forward model"; realistic noise can be included based on actual instrument characteristics. Potential systematic errors are difficult to deal with, and unexpected errors can surface after launch.

When possible, retrieval algorithms should be tested on data provided by existing satellites that are similar to the instrument of which the algorithm is being studied; e.g., for OMI algorithm testing, GOME data will often be used.

Some activities common to all of the Aura instruments will be undertaken with respect to simulated retrievals. In particular, a common set of atmospheric profiles will be used for some of the retrieval tests, and test plans and results will be discussed as part of the Aura Algorithm Working Group (and other Aura) meetings.

An overview of the planned algorithm testing activities for each of the Aura instrument teams is given below. The approach is given in the various Algorithm Theoretical Basis Documents. This activity would ideally be completed at launch and lead to "real-time" data with reasonably high confidence. However, the history of remote sensing has shown that reprocessing and algorithm changes or refinements can take place for years after launch, and each instrument team will have to deal with specific issues, all part of the validation process. Discussion in this document is limited to pre-launch algorithm activity plans, given that it is not possible to predict the extent and type of algorithm-related activities required after launch.

For details beyond those provided below, the Algorithm Working Group (chaired by Nathaniel Livesey, JPL; e-mail livesey@mls.jpl.nasa.gov) should be consulted.

4.2.1 HIRDLS Algorithm Testing

Evaluation and Testing

The evaluation and testing of HIRDLS science algorithms is an on-going process that commenced with early exploratory studies and will continue through post-launch data product validation. An example is the retrieval algorithm suite included in research codes (used for error analysis and sensitivity studies); in prototype retrieval codes (for processor engineering and development activities); and in delivered production software (for data product creation). It is also important to remember that often a hierarchy of algorithms may exist to do the same type of computation. This is particularly true in the area of the forward radiative transfer model where algorithms range from very accurate physical models necessary for precise calculations to computationally fast, highly parameterized codes for use in production processing. Inter-comparisons between the various members of the hierarchy provide important verifications as to the accuracy and robustness of science algorithms within the production environment. In the pre-launch period and at times during the post-launch period, data simulation provides an important mechanism by which algorithms can be evaluated with known, controlled inputs.

Test Configurations

Research codes represent the initial application of most science algorithms. It is within this context that potential algorithms are evaluated and tradeoffs are made. Thus research applications most often possess a degree of generality not always found in production algorithms. Prototype production algorithms represent a step toward a more constrained, science data processing environment. For HIRDLS, prototype science algorithms are delivered by the Science Development Group to the Data Product Development Group. These codes may not possess all of the attributes of final production codes and may fail to conform to language standards, coding standards and error handling requirements. In addition, the codes may not have undergone significant optimization by the science developers. Prior to delivery, prototypes will be verified as scientifically correct by the Science Development Group. The Data Product Development Group will test the codes for functional correctness within the context of the production environment. The Data Product Development Group will re-engineer the science prototypes into production codes as necessary. Evaluation and testing will encompass the entire processor units of which science algorithms are components. Evaluation criteria will emphasize functional correctness, completeness, robustness and efficiency. Testing will require a variety of simulated input data sets in the correct formats and with content appropriate to the goals of the various tests.

Simulated Observations

The various test approaches discussed in the previous section imply requirements for different types of simulated data. Research codes can often suffice with simple parametric data simulators. These may be off-line or in some cases are built directly into the research application. Detailed testing of production processors on the other hand require comprehensive simulators which can produce data streams that appropriately mimic the flow of actual data from the ground system. The needs for comprehensive simulated data sets arise from requirements additional to the development of production software components and include:

- verifying functional correctness and exception handling in the production environment.
- tuning processor performance and verifying resource utilization.
- performing end-to-end testing of the overall ground system.
- developing auxiliary software to support quality assurance and validation efforts.

Certain realities must be considered when developing a test and simulation philosophy. A comprehensive simulator can be very complicated and, as a consequence, potentially becomes a source of error itself. It is simpler and more cost effective to develop individual simulators for each data product level and thus provide test data that realistically represent situations stressful to the algorithms. This requires that the data interfaces be well defined, maintained and verified to assure that end-to-end flow through the processor chain will be successful. The HIRDLS team will produce a hierarchy of data simulators as part of the Science Data Product development activity. A key activity is the development of a database containing a variety of global scale atmospheric state parameters to be sampled at HIRDLS measurement points. This requires a simulator that can emulate the Aura spacecraft orbit as well as the HIRDLS scan pattern. The resulting atmospheric parameter profiles can then be used to calculate simulated observed radiance profiles in a Level-1 product simulator or formatted directly into a simulated Level-2 data product. Finally, the Level-1 product can be reverse-engineered into simulated Level-0 data. Assuming that appropriate care is taken, the various data products will be consistent and will allow processors to be tested individually or in an end-to-end manner.

4.2.2 MLS Algorithm Testing

Three major milestones are planned for the MLS retrieval software, roughly a year apart: the first major version mainly tests interfaces with external inputs, the second version implements most first-order features expected for accurate retrievals, and the third version is the “launch-ready” version; see Waters (1999) for a top-level schedule of the MLS data processing milestones.

For the purposes of pre-launch validation, the MLS team plans to perform simulation studies using the launch-ready software (and prior software versions), in order to assess the quality of closure for the retrieval processing suite; this pre-launch ‘algorithm validation’ leads to an important (and hopefully small) component of the final product uncertainty estimates, but it says nothing about the quality of the inputs used in the forward/retrieval model. These simulations include certain assumptions about the representation of the atmospheric profiles and the viewing geometry, in addition to a numerical representation of the radiative transfer and instrument and spectroscopic parameters (this numerical treatment is represented by the forward model, see Read [1999]). Optimum estimation methods are used for the retrievals, including the effects of non-homogeneity of the atmospheric state along the line of sight [Livesey and Wu, 1999; Livesey and Read, 2000]. Analysis of these simulations will involve many members of the EOS MLS team, and the results will be documented in terms of the quality of profile closure (comparisons of ‘true’ atmospheric profiles versus retrieved profiles), and quality of radiance closure (comparisons of simulated ‘observed’ input radiances versus calculated radiances based on the retrieved profiles, along with ‘chi square tests’). These simulations will be performed both with and without simulated radiance noise. Simulations will be performed using model atmospheric profiles from various sources (e.g., UGAMP test model, provided by R. Harwood; the common test case from MOZART model) to calculate forward model radiances, and perform retrievals for comparison to the original temperature and constituent profiles. Conditions for success are that good closure be obtained for all products using computer resources that would allow for daily processing and reprocessing of the MLS data. “Good closure” is defined by rms differences from the “true” profiles that are within a few percent, or radiance closure that is within the rms noise expected from the measurements. This type of closure exercise is a necessary condition for successful algorithm validation. Other errors can still arise when “real” radiances are used. Through these time-consuming exercises, retrievals can be improved, computer resources can be assessed, and “numerical” uncertainties can be estimated. Simulations and retrievals with increasing degrees of complexity and “realism” will be carried out (from crude tests to sophisticated two-dimensional tests for “small-scale” atmospheric features, with increasingly more realistic instrument parameters in the forward model).

Some comparisons of forward models between the JPL and University of Edinburgh members of the MLS team are also expected.

4.2.3 TES Algorithm Testing

End-to-End Closure Experiments

End-to-end closure experiments using the TES reference and operational software are used to test the robustness of TES level 2 retrieval algorithms and the operational software, and to identify problems either in the algorithm or in coding. These experiments will also be helpful for algorithm validation. A single step end-to-end simulation is to add noise to the model radiance and then to execute a step retrieval as defined in the TES Level 2 ATBD. A full end-to-end closure experiment is to generate a full global survey set of radiances with added noise and clouds and then to carry out the complete retrieval processing.

Establishing a profile/parameter database which consists of collections of measured atmospheric temperature and constituent profiles and surface parameter data by all means of observations, sonde, balloon, aircraft, satellite, etc. is one of the key activities for the pre-launch closure experiments. These profiles/parameters along with model simulated profiles allow us to compile the baseline initial guesses and the *a priori* , to simulate the observed spectral radiance, and to evaluate the retrieval results for all the possible atmospheric conditions including extreme cases. Global cloud coverage data will also be obtained so that the simulated TES global measurements will be more realistic.

The end-to-end closure experiments will follow three procedures: (1) simulate the TES observations using collected measurement profiles/surface parameters/cloud coverage as the true atmospheric full state with added noise, (2) generate TES retrieval products using a defined initial guess, and (3) examine and evaluate the retrieval results and error analysis by comparing with the “smoothed true profiles” and their statistical variance. Since the Level 2 software will be developed in steps from a single profile retrieval to automated full global survey data retrieval, the end-to-end experiment can be performed at each step.

Validation

Validation, in the sense used here, differs from validation of the TES geophysical measurements in that we will use pre-existing data that have already been analyzed by others. The objective is to ensure that the TES algorithm either produces identical results or there are plausible reasons why it does not. See section 5.1.3 for more details regarding TES Level 1 data validation.

4.2.4 OMI Algorithm Testing

Validation and testing of the algorithm are essential steps in the algorithm development. Validation of the algorithm has the objective to test if the developed algorithm produces data products within the required accuracy for that product as defined in the *Science Requirements Document for OMI-EOS* [Levelt et al., 2000a]. This is followed by tests of robustness, efficiency, completeness and functional correctness of the algorithm software. For OMI algorithm validation and testing are planned for the Level 0 → 1B, 1B → 2 etc. algorithms.

Validation of the Level 0 → 1B software will be done using the OMI-simulator software. With this tool it is possible to calculate Level 0 data from a given simulated high resolution (ir)radiance spectrum. Running the Level 0→ 1B software on the generated Level 0 data the original should be reproduced on the spectral resolution and sampling of OMI. Instead of using a simulated spectrum, it is also envisaged to start from calibration data, for example white light source and spectral line source measurements.

In the *GDPS Verification and Validation Plan (PL-OMIE-7000-FS-304, Schenkelaars 2000)*, testing of the Level 0 → 1B software is described. The tests cover all requirements from the User Requirements Document (REF) regarding robustness, efficiency, completeness and functionality of the software. Robustness tests of the software is envisaged with Level 0 data with predefined errors. Both validation and robustness tests will be done for several different orbits, reflecting (ir)radiance at all parts of the globe, for all seasons and for different atmospheric situations.

For the Level 1B → 2 algorithms the required accuracies for the Level 2 data are defined with respect to synthetic data [Levelt et al., 2000a]. The estimated absolute accuracy is the global root-mean-square difference between retrieved values and simulated "truth". Here, "truth" is defined as the input value of the product used in the radiative transfer model to generate measured and calibrated theoretical Earth radiance spectra. By validating the algorithm it can be checked if the requirements are met. This will be done with synthetic radiance and irradiance data sets which are as realistic as possible, using a state-of-the-art radiative transfer model and an accurate OMI simulator. The input for the synthetic data set generation should cover realistic atmospheric profiles, including clouds and aerosols, and should cover all parts of the globe for all seasons. The algorithms will be applied to these synthetic data.

Two synthetic data sets will be used. The first synthetic data set is provided by the algorithm developers. The main purpose of this limited data set is to perform validation of all sub-parts of the algorithm. The second data set will be provided by the OMI US team leader. This data set should cover several orbits of synthetic OMI data. With this data set an end-to-end test will be performed. The requirements stated in the Science Requirements Document for OMI-EOS will be checked using this data set. Also, the robustness of the algorithm will be tested, using Level 1B data with predefined errors.

Existing satellite data from GOME and SCIAMACHY will be used to do both algorithm validation and algorithm testing. Since the spectral resolution, wavelength range, spatial resolution and signal-to-noise ratio of OMI differ from those of GOME and SCIAMACHY, software has to be developed to produce quasi-OMI Level 1B data from GOME and SCIAMACHY Level 1B data. Comparing Level 2 products of GOME and SCIAMACHY with the Level 2 products derived from the quasi-OMI data should give an indication of the quality under realistic conditions. Also, the robustness can be tested in this way under realistic circumstances. Note that even preliminary product validation is possible with the Level 2 data produced from the quasi-OMI data, by comparing the products to correlative data sets.

Another method for algorithm validation is to compare different products that derive the same geophysical quantity. Within the international OMI science team, different methods for the retrieval of ozone column densities, aerosol optical thicknesses, and cloud height and cloud fraction are being developed. The results of these methods will be critically evaluated through intercomparisons.

4.3 Spectroscopic Data and other Databases: Needs, Priorities, and Plans

4.3.1 Spectroscopic Data

4.3.1.1 Spectroscopic Data for HIRDLS

The accuracy of the HIRDLS retrievals will depend, in part, on knowledge of spectral line parameters, heavy molecule cross sections, and aerosol refractive indices for the different channel target and interfering species. These quantities form a primary input to the forward model and the full simulation of the measurement process. The HIRDLS accuracy requirements for temperature (1 K absolute) and for constituent concentrations (5-10% absolute) are exacting. Note that inadequate spectroscopic knowledge is only one of many potential sources of error, so that the error budget for spectroscopy is considerably less than that represented by these figures. HIRDLS is a radiometer with channel passbands 10-50 cm^{-1} wide and the integrated channel radiances often contain the emissions from several gases whose contributions must be separated out by the forward model used in the retrieval. This requires high confidence in the spectroscopic parameters that are known and requires that there be no unknown emitters.

Table 4.1 lists the general spectroscopic parameter accuracy requirements for HIRDLS. For the most part, these are the same as for TES. The relative importance of parameters is also indicated (with 1 meaning highest priority).

Table 4.1. General requirements for HIRDLS spectral parameters.

Parameter	Desired Accuracies			
	Line List	Cross Sections	Importance Level	Concern?
Positions	0.002 cm^{-1}	0.01 cm^{-1}	3	NO
Intensities	3 %	5 – 10%	1	YES (XSections)
Pressure-broadening	5 %		2	YES
Pressure-shifts	0.002 cm^{-1}		3	NO
Temperature Dependence				
Widths	15 %		2	YES
Pressure shifts	20 %		3	NO

Compared to a high-resolution interferometer such as TES, HIRDLS uses relatively broad passbands. Line positions are therefore important, not so much in an absolute sense, as in the relative positioning of one line relative to another. Since lines of a given gas in a particular spectral region usually come from the same set of measurements, this implies an accuracy requirement for line positions of one gas relative to another in the same HIRDLS channel. Line positions and pressure shift effects are generally sufficiently accurate at this time not to compromise the HIRDLS retrievals.

Intensities receive the highest priority for accuracy. For the species that will be measured by HIRDLS, those for which line data will be used are generally already close to, or better than, the required accuracy level. There is a greater concern for the accuracy of the intensities of the heavy molecule cross-sections that will be used for those species for which line data is not available. To be useful for forward model calculations, cross-section data must be measured in the laboratory over the range of pressures and temperatures that are found in the atmosphere. HIRDLS will make high vertical resolution of the scientifically important region near the tropopause where temperatures often fall below 200 K. This is a potential problem since the quality of the cross-section data, where it exists, is generally poorer at lower temperatures.

The same considerations apply to the air-broadened widths and their temperature dependencies. These are the line parameters that are in most doubt at this time, even for strong absorbers such as water vapor.

All the instruments on Aura will make extensive use of the HITRAN database managed by L. S. Rothman at the Harvard-Smithsonian Center for Astrophysics. This is, in effect, the central international repository for spectral data and associated products that are also required by Aura such as aerosol refractive indices and partition sum parameterizations. Support for the management of this database, along with the quality control required for the inclusion of new data as it becomes available, is a high priority.

The main concerns for HIRDLS spectroscopy at this time and the prospects for improvements may be summarized as the following:

1 Improved H_2O widths and temperature dependencies are needed in all spectral regions. This is a recently funded activity and improvements should be in place by the time of Aura launch.

2 Cross-sections for $ClONO_2$ and N_2O_5 near 7.8 microns along with temperature and pressure dependencies that cover the full range of expected atmospheric conditions. These are the bands that HIRDLS will use to retrieve these constituents and if the data are not improved, the HIRDLS measurements could be compromised. These species also contribute significantly to the signal in the N_2O and CH_4 channels and if their emissions cannot be accurately quantified, they could also impact the retrieval of these two important tracers. Improvements are unlikely unless new laboratory measurements are made. We know of no such plans at this time.

3 HNO_3 parameters for both the 7 and 11-micron bands need improving. The former requires considerable work. Not only is this important for HNO_3 retrievals, but it could significantly affect the accuracy of the N_2O, CH_4, and $ClONO_2$ retrievals. This will require a combination of laboratory and theoretical spectroscopy. We are not aware of any plans to carry out this work.

4.3.1.2 Spectroscopic Data for MLS

MLS Needs for Spectroscopic Data

An accurate spectroscopic database is required for the retrieval of accurate geophysical products from MLS, since such data are likely to contribute in a major way to the overall accuracy of the end products. Spectroscopic data of interest are the emission line positions for all lines contributing significant signal in the spectral regions covered by the MLS spectrometers, the corresponding linewidths, and their temperature and pressure dependence. In addition, it is necessary to have accurate information about the continuum emission that affects the MLS measurements increasingly at lower stratospheric and upper tropospheric altitudes.

While a database exists for essentially all the required components [Pickett et al., 1992], along with some updates [e.g., Oh and Cohen, 1994], improvements will be made in both continuum and spectral line data. Continuum absorption is not adequately explained by line-by-line models; this includes absorption between lines or near (but several linewidths away from) a given line where the line absorption model (e.g., Van Vleck Weisskopf) fails. The absorption is expected to have a squared pressure dependence. The greatest needs are for continua from air (21% oxygen and 79% nitrogen) and water vapor (broadened by air). The continuum is needed between 175-208 GHz, 229-251 GHz, 631-669 GHz and 2500-2543 GHz. The air and water continuum near 118 GHz, although desirable, is less important because the 118 GHz O_2 line emission dominates. This knowledge is important for accurate retrievals. The minimum retrievable altitude for tropospheric water vapor will be estimated from the absorption baseline (what is left over after the line contribution is removed). The absorption baseline is the atmospheric continuum, which depends on moisture, temperature and pressure. The continuum adds opacity to the atmosphere. Accurate constituent retrievals in regions where the concentration is falling depend critically on getting the background absorption correct. Even though this absorption can be retrieved in theory, in practice there is always an issue of unknown instrument versus background atmospheric contributions which are not easily separable, because neither has a distinctive spectral shape. Plans are in place to perform the continuum measurements near 200 GHz in the laboratory at Ohio State University (F. De Lucia) and the continuum measurements near 2.5 THz at JPL.

The current status of EOS MLS molecular line spectroscopy is given in Table 4.2, along with the priority that we have assigned to each measurement of linewidth (and temperature dependence); spectroscopic priorities are also summarized in the next section.

All the electric and magnetic dipole moments for the primary MLS molecular suite are known and the spectra are well characterized. The line positions, strengths, partition functions and ground state energies are 1% accurate or better. This should not be a limiting source of accuracy. Some line positions of the EOS MLS constituent suite are unmeasured; these are italicized in Table 4.2. A greater source of uncertainty is the broadening parameter which characterizes the line shape. Of interest here is the collision broadening parameter. The Doppler broadening width is well known for all these molecules since it only depends on frequency, temperature and molecular mass.

Table 4.2 lists collision broadening measurements in air (79% N_2 and 21% O_2) for the specific line frequency. If the broadening can be estimated accurately from the existing database, this is given in italics in the table. Many of these molecules have collision broadening measurements for different lines or perhaps N_2 only. These are not listed in the table. The far right column lists the priority of the measurement: 1 means "most valuable," 2 means "very valuable," and 3 means "valuable;" a blank indicates that the laboratory measurements are already considered adequate. If no measurement is made, the collision broadening parameter will be guessed. The collision broadening parameters for most molecules are similar, within a factor of two, and approximately scale by the dipole moment. The temperature dependence is typically about 0.75. An educated guess should provide a collision broadening parameter that is adequate for a profile with about 10% accuracy, except for the lowermost altitude part of a decreasing profile (e.g., for ozone in the lower stratosphere), since systematic errors tend to amplify under these conditions. Linewidth measurements are challenging because sources of systematic errors are not always well understood. Typical laboratory work is probably worse than 5% accurate. Careful laboratory linewidth measurements are often reported to 1% accuracy, but intercomparisons among the best laboratory measurements typically agree only to within 3%. Therefore, 3% is arguably the best we can hope for regarding linewidth accuracies at the present time. A lower than 3% uncertainty in the table indicates where the laboratory measurement uncertainty is stated to be less than 3%. Often, there is a need for widths better than 3% but if a good < 3% measurement exists, these molecules are not considered priority measurement needs. In many cases, we feel that the linewidths need to be measured, as indicated in the table with priority 1-3.

Lines which may be used for MLS pointing information require an especially accurate linewidth. A 1% linewidth error is roughly equivalent to a 70 m error at the tangent point. We would like to obtain a pointing accuracy less than 10% of the retrieved profile grid spacing (about equal to the best MLS FOV width), or about 130 m. Therefore a 2% accuracy is desirable for those linewidths. Comparable accuracy already exists for the O_2 lines near 119 GHz, the main source of pointing for MLS stratospheric retrievals. The 240 GHz $^{18}O^{16}O$ line provides pointing and temperature information for the troposphere, and this linewidth has not been measured. The 625 GHz ozone line should be measured because it provides an independent pointing reference for that radiometer. The THz antenna scans independently of the other (GHz) antenna and relies on establishing pointing from O_2 and O_3 emission at 2.5 THz. Linewidth parameters for these molecules need to be measured (the 2.5 THz O_2 linewidth has been measured, but its accuracy is only 10%, and no temperature dependence measurement exists).

The satellite-based OH measurement is unique to MLS. There will be a limited set of opportunities to validate the OH profiles, mainly via infrequent aircraft and balloon-based OH measurements. Also, OH values decrease rapidly in the lower stratosphere, making these measurements a challenge. Therefore, the OH linewidth is a high priority measurement. One of the OH lines has already been measured; this should be cross-checked when the unmeasured line is done. Also, a nearby H_2O line width is needed to improve the radiance fit.

Upper stratospheric HCl determines the chlorine loading of the atmosphere, and it is important that this measurement is as accurate as possible. Existing HCl linewidth data include broadening by N_2 but without temperature dependence for the 626 GHz line measured by MLS; laboratory data on O_2 and N_2 broadening with temperature dependence at 2.5 THz also exist. With this data, one can estimate the air-broadened linewidth at 626 GHz within about 5%, but we would like to do better.

The linewidths for four strong ozone lines near 240 GHz are also needed, since these limit the accuracy for the MLS upper tropospheric ozone retrievals, which are challenging, particularly in the tropics. Systematic errors must be kept to a minimum, so very good linewidths are needed for these lines. The listed widths are estimates from a database of measured ozone widths.

MLS Priorities for Spectroscopic Data

The list of desired improvements in spectroscopic data for MLS measurements is summarized below, with priorities of 1 (most valuable), 2 (very valuable) and 3 (valuable). Conditions representative of the upper troposphere and stratosphere are required (temperature range of about 180 K to 300 K). First-order reasons for the desired improvements are also given.

(1) Most Valuable

Better laboratory measurements and theoretical expressions for water vapor continuum and dry air continuum absorption at frequencies between 100 and 2500 GHz (with desired accuracy of 5% or better):

(1a) At 175-208 GHz, for (improving the accuracy of) tropospheric humidity

(1b) At 229-251 GHz, for upper tropospheric ozone and tropospheric humidity

(1c) At 631-669 GHz and 2.50-2.54 THz, for improved constituent retrievals at pressures greater than ~ 50 hPa

Linewidth parameters, including temperature dependence (with desired accuracy of 3% or better) for:

(1d) 2.5 THz lines, namely OH (2 lines), O_3 (2 lines), O_2 (2 lines), O_2 (1 line), and H_2O (1 line), for improving the accuracy of OH retrievals

(1e) HCl (at 626 GHz), for accuracy of stratospheric chlorine loading

(1f) O_3 (4 lines at 230-248 GHz and 1 line at 625 GHz) and $^{18}O^{16}O$ (at 233 GHz), for accuracy of ozone retrievals

(1g) HO_2 (lines at 650 and 660 GHz), for HO_x chemistry

(1h) BrO (lines at 625 and 650 GHz), for stratospheric bromine loading

(2) Very Valuable

Linewidth parameters, including temperature dependence (with desired accuracy of 3% or better) for:

(2a) HCN (lines at 650 and 660 GHz), for upper tropospheric tracer data (and O_3)

(2b) CO (line at 230 GHz), for upper tropospheric tracer data (and O_3), comparisons with TES

(2c) HOCl, for chlorine chemistry

(2d) CH_3CN (lines at 184, 202, 625, 626, and 661 GHz), new global retrievals, recently demonstrated by UARS MLS

(2e) O_3 (additional lines at 231, 239, 248, and 250 GHz)

(3) Valuable

(3a) Linewidths and temperature dependence (with desired accuracy of ~5%) for SO_2 (lines at 200 GHz and ~660 GHz), for volcanic SO_2 plume studies

(3b) Linewidths and temperature dependence (with desired accuracy of ~3%) for O_3 (additional lines at 244 and 248 GHz)

(3c) Water vapor and dry air continuum absorption data at 113-122 GHz (with desired accuracy of ~5%)

Plans for MLS-related Spectroscopic Data Measurements

Plans are in place to meet the above spectroscopy needs for EOS MLS through laboratory measurement efforts underway at JPL (Ed Cohen and Brian Drouin) for linewidth parameters, and at Ohio State University (Frank DeLucia) for continuum data.

The schedule for these measurements is as follows:

- 600 GHz region
  - Transitions to be measured in order as follows: HCl, BrO, O_3, HO_2, and HOCl. HCl is completed, BrO and O_3 are nearly completed.
  - HO_2 measurements are in progress.
  - All but CH_3CN (deferred as it involves multiple lines of different widths) to be completed by end of December, 2001.
- 200 GHz region (and below)
  - $^{18}O^{16}O$ line at 233.9 GHz requires some new hardware and repeated measurements; planned completion is by end of March, 2002.
  - O_3, CO, and HCN combine for 11 features; planned completion is by end of June, 2002.
  - CH_3CN lines to be measured in parallel with 2.5 THz work (in 2002).
- 2.5 THz region
  - Some technology developments are needed (in 2001/2002).
  - Planned completion of spectroscopic measurements is end of April, 2003.

Most, if not all, of the EOS MLS spectroscopic needs are therefore expected to be met prior to mid-2003 and in time to incorporate into launch-ready software (forward model).

Table 4.2. Linewidth parameters for spectral lines targeted by MLS. Linewidth $w = P\ \gamma\ (300/T\ )^n$. Frequencies are italicized if not measured (uncertainty estimates in parentheses, in 0.0001 GHz). Current values for linewidth coefficients are indicated (and italicized if based on other related lines). MLS needs for measurements of γ and n are prioritized in last column (1: "most valuable", 2: "very valuable", 3: "valuable"; blank: adequate knowledge exists).

Molecule	**Frequency (GHz)**	**Pressure Broad.Coeff. γ (MHz/hPa)**	**Temperature Dependence Coefficient *n***	**Linewidth Function Accuracy[1] (%)**		**Priority**
				Current	**Desired**	
^{81}BrO	650.179 [2]				3	1
	624.768 [2]				3	1
CH_3CN	183.9 [2]				3	2
	202.3 [2]				3	2
	624.8 [2]				3	2
	626.4 [2]				3	2
	660.7 [2]				3	2
ClO	204.352 [2]	2.529	0.62	3	3	
	649.4512 [2]	2.087	0.86	3	3	
CO	230.5380				3	2
HCl	625.9188	*2.61*	*0.74*	5	2	1
HCN	177.2612				3	2
H_2O	183.3101	3.120	0.76	< 3	3	
	2531.9178				3	1
HOCl	635.8700 (1)				3	2
HNO_3	181.5496	3.272	0.75	3	3	
HO_2	*649.7015(0)* [2]				3	1
	660.4857 (0) [2]				3	1
N_2O	200.9753 [2]	2.430	0.87	5	5	
	652.8338 (0) [2]	2.300	0.75	5	5	
OH	2514.3167 [2]	2.652	0.74	3	2	1
	2509.9490 [2]				2	1
O_2	118.7503 [2]	1.644	0.74	< 3	2	
	2502.3239 [2]	1.28	*0.75*	10	2	1
$^{18}O^{16}O$	233.9462				2	1
O_3	206.1320	2.168	0.75	< 3	2	
	231.2815 (0)	*2.300*	*0.76*	5	3	2
	235.7098	*2.290*	*0.76*	5	2	1
	237.1462 (0)	*2.300*	*0.76*	5	2	1
	239.0933	*2.280*	*0.76*	5	3	2
	242.3187 (0)	*2.310*	*0.76*	5	2	1
	243.4537	*2.310*	*0.76*	5	2	1
	244.1580	*2.200*	*0.76*	5	3	3
	247.7618	*2.130*	*0.76*	5	3	3
	248.1834	*2.270*	*0.76*	5	3	2
	249.7886	*2.390*	*0.76*	5	3	2
	249.9620	*2.310*	*0.76*	5	3	2
	625.3715 (1)				2	1
	2509.5604 (5)				2	1
	2543.2084 (3)				2	1
SO_2	204.2468	2.92	0.78	3	3	
	200.2875				5	3
	660.4727 (0)				5	3
	660.9183				5	3

[1] Accuracy is for the linewidth function in air, 180K to 300K. [2] There are multiple lines near the listed frequency.

4.3.1.3 Spectroscopic Data for TES

Table 4.3. General requirements for TES spectral parameters

Parameter	Desired Accuracies	
	Line List	Cross Sections
Positions	0.002 cm^{-1}	0.01 cm^{-1}
Intensities	3 %	5 – 10%
Pressure-broadening	5 %	
Pressure-shifts	0.002 cm^{-1}	
Temperature Dependence		
Widths	15 %	
Pressure shifts	20 %	

The accurate retrieval of geophysical parameters from TES radiances depends critically on the accuracy of spectral databases containing line positions, line strengths, and their pressure and temperature dependencies. The general requirements for spectroscopic data for TES are listed in Table 4.3. The primary source of this information is the HITRAN Spectroscopic Database (Rothman et al., 1998) which contains both line parameters and cross sections. The line parameter species are reasonably complete but TES would benefit from improvements in pressure broadening coefficients (widths and shifts) and their temperature dependence for H_2O, CO (1-0 and 2-1 bands) and the 6.2 µm band of NO_2. In addition, existing improved measurements of spectral parameters for H_2O, O_3, CH_4, CO, NO_2, NO, N_2O, HNO_3, C_2H_4 (ethylene) and HCOOH (formic acid) should be collected, assessed and compiled into HITRAN format.

Adequate data for many cross section species exist, but are not included in the HITRAN database. Assessing and assembling this data into a TES standard cross section format is an important ongoing activity of the TES Science Team. However, cross section data for some important species are either inadequate or non-existent. New cross section data, including their temperature and pressure dependence, and air broadening coefficients are needed for PAN (peroxyacetyl nitrate) and PNA (peroxynitric acid) between 650 and 2500 cm^{-1}, and for acetone (CH_3COCH_3) and acetic acid (CH_3COOH) between 650 and 2000 cm^{-1}. Although of lower priority, TES would also benefit from improved cross section measurements of methanol (CH_3OH) and methyl hydroperoxide (CH_3OOH).

Any new measurements of aerosol infrared spectral properties would also benefit TES.

4.3.1.4 Spectroscopic Data for OMI

The list of desired improvements in spectroscopic data for OMI measurements is summarized below, with priorities of 1 (most valuable), 2 (very valuable) and 3 (valuable). The current status, including references to literature spectra, is also summarized.

The UV/VIS absorption spectra of the molecules measured by OMI (O_3, NO_2, SO_2, BrO, OClO, and HCHO) will be included in HITRAN 2000.

(1) Most Valuable

OMI retrieval algorithms rely on accurate temperature dependent absorption cross sections of the molecules studied on refractive indexes of aerosols (especially desert dust aerosol in the UV) for the derivation of the aerosol spectral optical thickness, and on accurate Ring spectra, needed to correct for the Ring effect that fills in absorption lines in the terrestrial spectrum. Since the assessment of cloud height is important for the retrieval of other species, O_2-O_2 absorption spectra and rotational Raman line strengths of N_2 and O_2 need to be known accurately. The current status and spectroscopy needs are described below:

O_3: The available reference spectra in the UV/visible are not satisfactory. The Bass & Paur temperature dependent cross sections [Bass & Paur, 1985] have been re-calibrated in wavelength, these will be included in HITRAN 2000. Whether to implement the re-calibration for OMI is under discussion. Further FTS measurements of ozone spectra are strongly encouraged.

O_2-O_2: The agreement between various published cross section spectra is not satisfactory. The temperature dependence is not clear [Greenblatt et al., 1990; Newnham and Ballard, 1998], and the peak absorption amount is uncertain by about 15 % [Perner and Platt, 1980 and references therein; Newnham and Ballard 1998, and references therein]. Measurements are necessary to better determine the absorption spectra as well as their temperature dependence.

OClO: The available reference spectra [Wahner et al., 1987] need improvement, but it is envisaged that this will be achieved before launch.

SO_2: Good spectra are available at room temperature [Manatt and Lane, 1993]. The need for additional low temperature measurements is to be determined, depending on the outcome of measurements (by J. Halpern) to confirm earlier measurements by McGee and Burris.

NO_2: The preferred absorption spectra to be used for NO_2 have been published for temperatures of 220 and 294 K [Vandaele et al., 1997], and measurements at 241 K are expected to be available soon [A.C. Vandaele, private communication]. Measurements at intermediate temperatures would be very valuable. A detailed study of the available spectra and their quality is being performed (by J. Orphal) and the spectroscopic data needs will depend on the outcome of that study.

(2) Very Valuable

H_2O: In the UV/VIS range, the best currently available spectra are HITRAN96 and a very complete spectral database by Michel Carleer and others at the Université Libre de Bruxelles. The H_2O data are currently being reviewed and will possibly be revised.

Solar spectrum: An extraterrestrial Fraunhofer spectrum would be very useful for accurate determinations of the Ring effect, as well as for other purposes (wavelength calibration, undersampling correction), but possibly synthetic Fraunhofer spectra will become available before the Aura-launch that can be used instead.

(3) Valuable

Ring effect: The rotational Raman line strengths of N_2 and O_2 need to be known accurately to correct for the Ring effect. The knowledge of the Ring effect is good, and knowledge of the Ring effect divided by the solar spectrum (as used in DOAS fits) is reasonable.

For the following species, there is currently no strong need for further spectroscopic measurements:

BrO: Wilmouth et al. [1999].

HCHO: Cantrell et al. [1990].

The needs and priorities for spectroscopic data are currently under review within the OMI team; we envisage that spectra will be included in HITRAN.

In addition, we are assuming that OMI Flight Model measurements of absorption cross sections convoluted with the OMI instrument transfer function (slit function and CCD pixel response function) will be made during the PI calibration period [Dobber, 2001]. These measurements are complementary to the much more accurate spectra described above, and are performed for the purpose of determining the instrument transfer function, and as an instrument performance check.

4.3.2 Other Databases

Some databases that will be of general use to the Aura instruments include:

- climatological data sets (or models); it is the responsibility of each team to provide their own climatological data sets.
- operational meteorological data (e.g., NCEP or DAO data for use in validation as well as in retrieval “a priori” or first-guess information)
- a database for accessing the correlative data (probably at the GSFC DAAC).
- predictor software to allow for detailed planning of correlative observations coincident with each of the Aura instrument viewing vectors; use of the Science Data Processing Toolkit should allow one to provide this type of information for any viewing vector.

4.3.2.1 Other Databases for HIRDLS

Aerosol and cloud particles may make a measurable contribution to infrared limb opacity in the region from the upper troposphere into the mid-stratosphere. Aerosol and cloud opacity has a slowly varying, but significant, wavelength dependence that depends upon particle composition (which determines optical constants), particle size distribution and particle shapes (spherical, columnar, bullet rosettes, etc.). Optical constants of atmospheric particles, in addition to compositional dependence, can have some measurable temperature dependence in the infrared and in general have not been as well characterized by laboratory measurements as gas-phase molecular spectra have been.

There is a need for infrared spectroscopic data (optical constants) for a variety of solid and liquid atmospheric particle types including sulfate aerosols, polar stratospheric clouds, cirrus clouds and tropospheric aerosols. Currently, measurements of optical constants for sulfate (H_2SO_4/H_2O) aerosol mixtures exist, but there are large differences among laboratory measurements. The composition of polar stratospheric cloud particles remains uncertain but likely includes water ice, nitric acid trihydrate (NAT), nitric acid dihydrate (NAD), and ternary solution ($H_2SO_4/H_2O/HNO_3$) droplets.

There is also a need for databases that better define mid-latitude, sub-visible, and tropical cirrus cloud properties including typical particle sizes and shapes (possible temperature dependence), and their corresponding infrared scattering parameters. Of particular need is the single-particle scattering parameters, such as absorption and extinction coefficients, for non-spherical shapes; e.g. hexagonal, plates, rosettes, other crystal shapes.

CO_2 mixing ratio measurements are needed in the stratosphere for derivation of temperature. In addition, conventional meteorological analysis would also be useful.

4.3.2.2 Other Databases for MLS

Although the following data does not represent a “laboratory database,” it is worth pointing out that there are other types of “databases” relating to the atmosphere that would be valuable for improving the interpretation of EOS MLS measurements, in particular in relation to clouds. Scattering by high clouds (about 8 km altitude or higher) can affect the radiances for lower stratospheric and upper tropospheric MLS measurements, especially if thick cirrus clouds are present, with significant ice particle concentration at sizes larger than roughly the wavelengths detected by MLS measurements. Measurements to produce a climatology of the properties of tropospheric clouds above 8 km in altitude can be used to improve the retrieval of ice water content. These properties include the particle number density and size distribution, for particles larger than ~100μm, as well as information on total ice content. Correlative data of this kind are also needed after launch.

Climatological data sets and/or models will be used as part of the retrieval software for MLS products as a priori information which will help retrieval stability in regions of poor sensitivity, namely the highest and lowest portions of the retrieved profiles. Real-time information for temperature and tropospheric humidity will be used as a priori information with conservative error bars that are based on DAO data and/or NCEP data.

4.3.2.3 Other Databases for TES

In addition to the general climatological data, operational meteorological data, coincidence predictor, and correlative database needs mentioned above, TES will utilize a database of global land cover to aid in the initial estimates of land surface infrared emissivity. For algorithm development, and maybe initial operations, the U.S. Geological Survey (USGS) Earth Resources System Data Center global land cover maps will be employed. Later on, emissivity data will be taken from the ASTER instrument on the Terra platform.

4.3.2.4 Other Databases for OMI

Databases are needed for retrieval and for validation purposes. There are two types of databases: static and dynamic. Static data are those entries that are not frequently changed, such as spectroscopic data and climatologies. Dynamic data are frequently updated, for example cloud information or daily or weekly snow and ice data.

For OMI algorithm retrieval, the following static databases are needed:

1. Climatological databases.
2. Spectral surface reflectance databases.
3. Snow and ice coverage.
4. Terrain height.
5. High resolution solar reference spectrum.
6. OMI slitfunction.
7. Ring spectrum.

Dynamic databases needed for retrieval are:

1. Meteorological databases.
2. Data measured by other EOS-satellites like Terra, Aqua, ESSP3 (PICASSO-CENA), POLDER and CloudSat for obtaining cloud/aerosol information, snow/ice coverage, temperature or surface pressure information.
3. data from other satellites (e.g., ENVISAT) potentially improve retrievals by OMI but are not strictly necessary.

For validation purposes, static climatological databases may be used for a first order comparison. All correlative data sets that are used for validation are dynamic data sets. To overcome the problem of spatial and temporal mismatches between OMI data and correlative data sets, data assimilation codes have to be developed to interpolate correlative data sets in space and time.

4.4 Summary of Aura Plans for Pre-launch Activities

Three major pre-launch activities that are necessary for successful (post-launch) validation of Aura products are: (1) Instrument calibration, (2) Algorithm testing, and (3) Compilation of spectroscopic data and other databases. For the first two topics in particular, the purpose here is to provide some sense of direction and references to other documents and working groups, rather than detailed plans and/or schedules.

4.4.1 Instrument Calibration

Instrument calibration is closely tied to the continuing hardware development and testing of the Aura instruments. Each instrument will have detailed specific issues and schedules to follow. Pre-launch instrument and Project reviews and reports provide the means to assess the progress of the calibration plans that are briefly discussed (section 4.1).

4.4.2 Algorithm Testing

Pre-launch algorithm testing is discussed in section 4.2. The success of this testing directly impacts the quality of processed data after launch. Current test plans are summarized for each instrument team's algorithm. Where feasible, algorithms will be tested on data obtained by earlier satellite instruments. Algorithm mathematical approaches and some accuracy estimates are given in the Algorithm Theoretical Basis Documents. The Algorithm Working Group will guide some of the common activities (e.g., the use of a common model atmosphere for simulations and end-to-end testing), but much of the detailed work rests within each instrument team. Updates regarding algorithm status are ongoing and planned on a regular basis before the launch-ready software deliveries.

4.4.3 Spectroscopic Data and other Databases

Databases of interest to the Aura instrument teams are identified, along with needs for new spectroscopic data (section 4.3). Since spectroscopic data generally come from outside the instrument teams, such needs were recently included as part of a NASA Research Announcement towards validation of data from the Aura and Aqua platforms. Through this and similar efforts, it is expected that many of the desired improvements in these databases will be met before the Aura launch. However, some important items (notably, information on the challenging HNO_3 infrared bands of relevance to both HIRDLS and TES, and on O_2-O_2 visible absorption cross sections for OMI) will require more attention in order for the satellite measurement accuracy requirements to be met. As each instrument team stays abreast of the uncertainties that remain in these databases, proper estimates of expected post-launch accuracy in the retrieved geophysical products can be made; this is a crucial and time consuming aspect of the validation assessments.

Other pre-launch activities currently underway include the gathering and/or development of data sets for use in the retrievals and/or simulations (climatology, operational meteorological data, or model values), coincidence predictor software, as well as gathering of other databases such as surface albedo and emissivity.

4.4.4 Models

Atmospheric models have several pre-launch applications to Aura validation. Constituent fields from atmospheric models will be used in synthetic data needed for algorithm testing. These constituent fields will also be used to develop strategies to obtain optimal information from comparisons of correlative observations with Aura measurements, especially in the upper troposphere and lower stratosphere where temporal and spatial scales of variability are much smaller than in the middle and upper stratosphere. Model fields will be used to develop quantitative requirements for coincidence criteria and also to develop statistical methods of comparison.

5 Aura Plans for Post-launch Activities Relating to Validation

Post-launch validation activities include forms of validation and data quality assessment methods other than comparisons of retrieved quantities with correlative data. These studies are expected to continue for many years, including updates when Aura data sets are reprocessed. They include: assessment of instrument calibration and pointing, proper screening of bad data, routine inspection of incoming data and radiance residuals, and other planned analyses. An outline of plans for each instrument team is provided in Section 5.1 below. Details are left to future documents from individual Aura instrument teams particularly for many activities that are specific for each instrument.

Plans for geophysical data comparisons between Aura products and correlative data from a variety of sources are based on the discussion in section 5.2. Some specific details regarding these plans will await future decisions about funding for Aura-specific validation proposals, although some of the plans for correlative data collection, location, and dissemination will need to proceed well ahead of the Aura launch, soon after the first phase of this Validation Plan.

5.1 Data Quality Assessment Plans (other than correlative geophysical data or models)

5.1.1 HIRDLS Data Quality Assessment Plans

5.1.1.1 HIRDLS Engineering and Level 0 Data Quality Assessment

Procedures for assessing the quality of all of the data from HIRDLS will be implemented at all levels of the processing, and flags attached to the archived data will indicate the tests which have been done and any data which evidence a problem, either because of some instrument problem or some concern in the retrieval process.

Engineering data will be analyzed routinely to determine that parameters are within the acceptable range, to detect any trends that might indicate instrument changes that could presage a problem, and to determine the extent to which any variability in instrument state is affecting the science data. Parameters will be compared to values determined before launch and acceptable ranges of variation defined so that any excursions beyond these ranges will be flagged for special attention by the instrument team.

At level 0, radiometric data will be examined by simple checks for realism. Low order bits of the A/D output, for instance, should be equally probably zero or one. If a particular bit remains with only one value, it would be very suspect. For most channels the signals should be monotonically decreasing with altitude. Rapid oscillation or spikes in the signals would indicate a problem.

Level 0 signals are converted to level 1 radiances on the basis of zero radiance space view signals measured above the atmosphere and standard signals from the IFC measured at frequent intervals. These signals could change without obviously affecting the derived radiances, and still indicate a problem. Thus we will maintain files of the actual signals in these cases to examine for trends or offsets. For instance, if the sensitivity of a detector were decreasing or the reflectivity of the scan mirror were decreasing, the space view signal would not change much, but the IFC and atmospheric signals would be decreased proportionally. The level 1 derived radiance would be unchanged, but the actual IFC signal would indicate the problem. Similarly, a radiometric problem in the space reference channel would cause both space view signal and IFC signal to change, without affecting the level 1 radiances. One example of such a problem would be those rare times when the moon is within the view of the space reference channel.

We have the capability of returning data at a higher rate from a few channels. It will be useful to check occasionally the data at the chopper blade rate (500 Hz) instead of the chopper rotation rate (83 Hz) for consistency, and to see whether there are any periodic effects in the data being filtered out by the processing.

Noise levels for each channel will be measured in the space view and the IFC view, and compared to values from calibration before launch. Signal levels in the space view will be monitored as a function of azimuth angle, since variation in these could indicate contamination building up on the scan mirror, affecting the angular variation of its reflectivity. Occasional pitch up maneuvers will allow the determination of the angular dependence of scan mirror emissivity and this can be compared to the azimuthal variation of space view signals.

5.1.1.2 HIRDLS Level 1 Data Quality Assurance

Level 1 radiances will be compared with radiances computed before launch with model atmospheres created from climatology. This will indicate any gross problems with the radiances. Radiances can be compared for up and down scan directions to check for any systematic effects. For those species which do not vary significantly diurnally, comparison of radiances at the same location on ascending and descending nodes provides a valuable check, especially for any effects of short wavelength stray light.

Radiances will be correlated with instrument temperatures, sunshield position, and other engineering parameters to detect any effects outside the expected range.

In the tropics, there are relatively low horizontal gradients under most meteorological conditions. Comparison of successive scans here might indicate unexpected variability that could be related to instrument performance.

5.1.1.3 HIRDLS Level 2 and Level 3 Data Quality Assurance

Additional checks will be performed on the profiles of temperature, pressure, and mixing ratio produced by retrievals producing level 2 profiles from level 1 radiances.

The retrieval process itself produces several indicators of data quality. The standard deviation between the input radiance and the radiance from the forward model is indicative of the SNR of the data. These will be tracked for trend, and compared for consistency with the noise as measured in the space and IFC views. The frequency content of the residuals, especially the correlation among channels, provides information on pointing jitter. The number of iterations necessary for convergence of the retrieval and the percent of the retrieved quantity attributable to the a priori information also are useful indicators of data quality.

In the retrieved profiles, we will look for unexpected variations in tracer-tracer correlations, for instance CFC11-CFC12 and CH_4-N_2O.

At level 3, the variance in the data assimilation compared with knowledge about atmospheric variability can indicate systematic problems. Comparison of retrieved maps with climatology can indicate systematic effects (as well as discoveries!).

5.1.1.4 HIRDLS Assessment of Uncertainty

Assessment of data uncertainty is an important aspect of data validation. Uncertainties include both the imprecision due to random noise in the signals, as propagated through the retrieval process, and biases due to errors in instrument and retrieval parameters such as spectral response or molecular line parameters. Precision values can be generated from noise assessments of detector signals in the space and IFC views, and from pointing jitter; these can be used to evaluate the random error in the retrieved radiances, and from the radiance errors, estimates can be made of the random errors in the profiles.

Biases are more difficult to detect. For several species (CO_2, H_2O, O_3) we have redundant channels. We will compare the retrieved temperature and concentration profiles using different combinations of channels (over appropriate altitude ranges) for consistency to detect any errors in, for instance, the pointing offset of different channels or the spectral response. Biases between HIRDLS data and high quality validated correlative data, which contain their own errors, need to be understood in terms of the expected uncertainties in the respective data sets and other possible sources of error.

5.1.2 MLS Data Quality Assessment Plans

5.1.2.1 MLS Calibration, Pointing Assessment, and Level 1 Validation

Post-launch activities relating to calibration and pointing are an important part of the data evaluation. These activities include an analysis of engineering data from the instrument, in terms of instrument 'health' and a search for any 'trends' in these data (on an orbital or sub- daily basis, as well as on a seasonal, or longer-term basis). While we expect very good stability from the EOS MLS instrument (as was achieved for UARS MLS), certain conditions will be different (e.g. thermal environment around the orbit). Instrument status will be carefully monitored and documented. Some of the early on-orbit calibration plans call for some Aura pitch maneuver(s) to check for spectral baseline offsets and sidelobe levels in the field-of-view. The EOS MLS instrument also has the ability to perform spectral channel sweeps to ascertain whether any post-launch changes in filter position or shape occur over time.

Another post-launch calibration check involves the use of the moon as a calibration for pointing differences between the various radiometers (and as a check for possible post-launch shifts in the alignment for the EOS MLS antenna and radiometer system with respect to the satellite frame of reference). Such work was performed for UARS MLS, through the use of a thermal model of the moon and an estimation of the angles needed for a best fit between observed and calculated radiances at several different times during the mission [Jarnot et al., 1996]; similar studies will be planned for EOS MLS. Although the tangent pressure is retrieved during data processing of EOS MLS data, so that the alignment issues are not a first-order issue, relative shifts between radiometers could lead to some inaccurate assessments of pointing for some measurements, from radiometers that are not (heavily) used for tangent pressure retrievals. Another indication of pointing problems could come from comparisons between retrievals of the same atmospheric species from different radiometer bands (see section 5.1.2.5.1).

For Level 1 radiance validation after launch, the most direct comparison with similar radiances would be between EOS MLS radiances and UARS MLS values, if UARS MLS data are still being obtained in 2003. The ODIN microwave data would also provide some comparison possibilities if the instrument is operational in 2003. In either case, one would still expect some differences in the measured spectra, which would have to be reconciled (for exact frequencies, tangent heights, viewing angles, time of day, etc...). Radiance residuals between the EOS MLS radiances and the calculated (forward model) radiances will likely be the best indicator of potential problems in the calibrated Level 1 data, given that the forward model has proven to be quite accurate based on UARS MLS experience (with retrieval results being the ultimate test).

5.1.2.2 MLS Data Quality Controls and Diagnostics

Proper flagging of bad data (because of an instrument problem of some kind, or because of a retrieval problem) is a first needed step, as part of the software that generates the data products. We envision a plan similar to UARS MLS, where one 'status variable' was used to screen for the profiles that should have good input radiances (and a priori values), and another 'quality variable' was used to provide information about goodness of fit (at the radiance level), based on chi square tests [see e.g. Froidevaux et al., 1996, Waters et al., 1996, for a description of UARS MLS data screening – a condition that should be set to 'unusable data' only a small fraction of the time]. Another example of such necessary screens is under certain conditions of interference by, for example, the moon in the field-of-view. Flags will also be used for

EOS MLS to point out the likely occurrence of cloud interference, when this could be a problem for the data quality (see Livesey and Wu [1999] for a preliminary description).

All details regarding the plans for such routine analysis products and diagnostics for EOS MLS are not included here. We will plan for the above types of diagnostics, in order to more easily validate the EOS MLS data, even if this means 'throwing out' a small fraction of the data.

5.1.2.3 MLS Routine Data Inspection

The MLS team found that, for UARS MLS data, it was essential to examine all incoming data products to keep up with first-order data quality, and to check for software or instrument problems, especially during the first few months after launch. Routine data inspection will also be planned for EOS MLS data. For Level 1 data, plots of radiances and time series of engineering data are useful. For Level 2 data, we plan to produce plots showing the time series at all pressures for each product every day (at least initially); when some confidence is gained in the first-order data quality, fewer coefficients of the retrieved profiles need be routinely displayed. However, knowledge of the statistics of "spikes" is also very useful, and we plan to utilize such analyses and plots for EOS MLS Level 2 data. Estimated uncertainties will also be plotted, as another diagnostic of potential problem areas (where the uncertainties could increase significantly). Finally, zonal mean plots and daily maps (based on Level 2 and Level 3 data) will be produced; section 5.1.2.5.2 discusses comparison plots of the MLS data versus climatological and/or model values, which will be a useful part of routine data evaluation, especially in the early stages of the mission (when comprehensive comparisons with correlative data will not yet have occurred). Planning for such regular data inspections and organizing team meetings to share results will be a major activity, especially right after launch, and will continue through all reprocessing phases. The MLS team plans to organize and document these "inspection products" in advance of launch.

5.1.2.4 MLS Radiance Residuals

Closure ('within the noise') between observed and calculated radiances is a necessary (but not sufficient) condition for high quality retrievals. Thorough examination of such radiance residuals and related chi square tests for closure will be performed on selected days (at least for one day per week, during the early stages of the mission). Detailed analyses of this kind can point to certain imperfections in the assumed knowledge about certain instrument parameters, or even in spectroscopic parameters [e.g., Pumphrey et al., 1999]. Good radiance closure is not sufficient, however, since a 'zigzag' profile can produce essentially the same quality of radiance fit as a smooth one, but only an examination of the profile itself would reveal such an instability (a retrieved profile can 'overshoot' at a particular height to compensate for a problem at another height).

Radiance closure tests and global time series of chi square tests were useful during UARS MLS data analyses to point out certain regions of the atmosphere and certain time periods for which poorer fits occurred. Often, such phenomena can be understood in terms of poorer instrument performance or a more dynamic atmosphere. Such diagnostics will be produced for EOS MLS.

5.1.2.5 Other MLS Consistency Checks

MLS Retrieval Results from Different Spectral Regions

A feature of MLS retrievals that helps to provide some internal consistency checks is the availability of more than one spectral region for the independent retrieval of the same quantity (e.g. for ozone profiles). We plan to study the consistency between these 'diagnostic products' very closely, in order to assess whether the 'same atmosphere' is being retrieved (within the respective uncertainties) via these different means. An 'optimum' product will be produced for the outside users, based either on a combined retrieval from all spectral regions or on a preferred set of spectral regions, after pre- and post-launch analyses of this issue.

MLS Data Comparisons with Climatology

The EOS MLS team will compare the incoming geophysical data (Level 2 and Level 3) to climatological atmospheric data, based for example on UARS-derived climatologies, and, if no climatology exists, on atmospheric models (through the Edinburgh University access to such models, UGAMP in particular). Model atmospheres are necessary anyway for planning retrieval simulations prior to launch. Such checks are good for first-order assessment of the data quality and 'reasonableness,' especially in the first few weeks of the mission, when such comparisons can be performed faster and for a better 'global view' than through the use of correlative data.

MLS Assessment of Uncertainty Estimates

Another important validation activity is the assessment of data uncertainties. This includes random noise uncertainty, both at the radiance level (since these estimates are transformed into geophysical product precision estimates), where checks of precision can performed based on observed rms space radiance variability, and for the Level 2 products. Empirical precision values can be generated by computing rms variability in the retrieved profiles for conditions where true atmospheric variability is believed to be minimal (e.g. through the use of a narrow tropical latitude band, at least for the stratosphere, or through the use of observed differences between near-coincident profiles). Moreover, random error estimates from different satellite results or for other comparisons with enough statistical sampling can be checked for consistency against the rms variability in the differences between the data sets. This was done for some UARS validation studies. For accuracy, theoretical estimates of possible biases based on sensitivity studies, using the uncertainties in knowledge of spectroscopy, instrument parameters, and all possible sources of error, need to be reconciled with the final results from correlative data comparisons. Any biases between MLS data and high quality validated correlative data (which can never be errorless themselves) need to be understood in terms of the respective expected uncertainties between the datasets and other possible sources of error that were not accounted for (from instrument errors to forward model or retrieval errors, or possibly atmospheric effects such as cloud contamination, which ultimately are equivalent to a retrieval issue).

5.1.3 TES Data Quality Assessment Plans

5.1.3.1 TES Calibration, Pointing Assessment, and Level 1 Validation

The first activities following post-launch decontamination will be to perform a series of internal calibration sequences designed to measure on-orbit radiometric performance and test post-launch detector array alignment. Although the commanded angles of the gimbal pointing mirror rely heavily on pre-flight calibration, they are also verified during these tests. The instrument pointing angle is retrieved in Level 2, using the recorded angle as a first guess.

For internal consistency, radiometric calibration is tested by using the known Planck function for the on-board cavity blackbody calibration source at its recorded temperature. Using spectral measurements of the cold space view (for the instrument offset radiance) and the blackbody, we can perform calibration of separate blackbody spectra and check that they match the expected Planck functions. Once this is verified, we can proceed with calibration sequences that measure orbital variations in offset radiance and/or calibration slope and any changes to pre-launch characterizations of non-linearities, amplifier gain scale factors or interpolation functions for applying lower resolution calibration measurements to our higher resolution scans. These types of calibration sequences are performed as soon as possible after launch and as needed during mission operations.

A check of the noise equivalent spectral radiance (NESR) estimated from each spectrum using the out-of-band region can be performed by comparing the observed rms variability in several calibration measurements of the same cold space and blackbody source.

For checking detector array co-alignment, the on-board spatial calibration source is scanned by the pointing mirror. The spatial calibrator is an illuminated slit positioned parallel to the long axis of the detectors. Simultaneously recorded spectra are analyzed to test whether the expected pixel in each array was viewing the source. The results of these measurements are used in the retrieval algorithm to accurately specify pointing in the retrieval forward model. Also, the need to reevaluate the line shape function in-flight can be diagnosed by the characteristics of the residuals between the measured and modeled atmospheric spectra.

The TES Level 1 product is geo-located spectral radiance. Spectral radiance is the fundamental quantity from which all other data products are derived, and the accuracy of the radiance measurement is one of the major factors controlling the accuracy of all other data products. The validation of radiance is mainly a check on the calibration of the measurement system. That is, the primary function of calibration is to convert the instrument output (i.e., DN) to radiances. Radiance validation is a validation of the DN to radiance calibration process. The radiance measured at the instrument for nadir views contains contributions from surface emission, from surface-reflected downwelling atmospheric emission and from upwelling atmospheric emission. The relative contribution of each is strongly dependent on wavenumber, the state of the atmosphere, and the temperature and properties of the underlying surface. The challenge is to find a target where the three contributions can be accurately determined to permit an accurate estimate of the radiance at the instrument from earth bound measurements. For significant portions of the TES spectral range, nadir views of bodies of water on earth offer the most promise. Two advantages of water are that its emissivity is high and relatively constant in the TES spectral range [Masuda, et. al., 1988] (greater than 0.95 for nadir views), and there are bodies of water where the surface temperature is uniform over reasonably large areas. Candidate locations are the Gulf of Mexico and Lake Tahoe in California/Nevada. The Gulf of Mexico is attractive because satellite overpass opportunities are frequent. The advantage of Lake Tahoe is its altitude. This greatly reduces the uncertainty of estimating the atmospheric contributions to the top of the atmosphere radiances. The lake is also a major site for validations of the thermal IR channels of ASTER and MODIS on the Terra platform for which it has been highly instrumented.

A radiance validation requires several ground and aircraft based activities. The general approach has been described and demonstrated by Smith et. al. [1996]. It is imperative that the water surface temperature and emissivity, and the state of the atmosphere be known at the time of the satellite overpass. The surface temperature and emissivity are determined by a combination of down-looking and up-looking spectrally resolved radiance measurements near the water surface. Errors will be reduced if the spectral resolution of the surface radiance measurements is close to the TES nadir spectral resolution. Buoy based water temperature measurements over a large area are needed to support and verify the IR radiance measurements of water surface temperature. The atmospheric contribution is determined by sonde and aircraft-based spectrally resolved upwelling radiance measurements. The sonde must measure temperature, humidity and ozone. Multiple launches (e.g. before, during and after a platform overpass) would provide an assessment of atmospheric variability. Spectrally resolved measurements of the upwelling radiation from above 10 km provide a direct measurement of radiance. Measurements of Lake Tahoe from this altitude or higher capture much of the atmospheric opacity in several spectral regions and can be compared directly to the radiances measured by TES in the 10-12 µm window region.

Data sources currently identified that are (or will be) appropriate for radiance validation are:

(1) Airborne Emission Spectrometer (AES). AES operates in both a downlooking mode from a variety of aircraft and uplooking from the surface. It was specifically designed to cover the same spectral region at the same resolution as TES and is therefore a prime data source for validation exercises. Downlooking data are very similar to the TES nadir mode and uplooking data are a useful surrogate for TES limb data.

(2) AERI (Atmospheric Emitted Radiation Interferometer). AERI is a well calibrated, 1 cm^{-1} spectral resolution, uplooking, Michelson interferometer covering the range 550 to 1700 and 2000 to 2500 cm^{-1}. Several copies of the instrument are operational – the one of primary interest for TES validation is located at the Central facility of the ARM Cloud And Radiation Test (CART) site in northern Oklahoma. The AERI-X (eXtended resolution AERI) is also located at the central facility. It has 0.1 cm^{-1} spectral resolution, but only covers 550 to 1600 cm^{-1}. The ARM program provides good temperature and water vapor information about the atmosphere overhead. Information about ozone and other stratospheric gases, as well as aerosol optical depth, is available from solar absorption instruments at the site.

(3) HIS (High resolution Interferometric Sounder). HIS is an autonomous FTS that flies on the ER2 in a variety of campaigns with the goal of temperature and water vapor sounding. Some of the more recent campaigns have been in support of tropospheric chemistry missions, where independent measurements may also be available. Although the spectral resolution is lower, the data are from an altitude that is more "space-like" than the AES data.

(4) IMG (Interferometric Monitor of Greenhouse Gases). IMG, a nadir sounder developed by the Japanese, flew on the ADEOS mission (which failed in June 1997). Nevertheless, it represents the only source of real space-based data with spectral coverage and resolution very close to that of TES. Some tests using IMG data are already ongoing and more are planned.

(5) MIPAS (Michelson Interferometer for Passive Atmospheric Sounding). MIPAS will fly on the ENVISAT mission at least one year before TES. It is a limb sounder with slightly poorer spectral resolution than TES but will nevertheless be the only source of space-based limb emission data prior to TES, so it will be a very valuable validation tool.

(6) NAST-I (NPOESS Aircraft Sounder Testbed – Interferometer). NAST-I is a nadir-viewing instrument that has flown on several ER2 missions, including CAMEX-3, with correlative radiosonde measurements. It has a spectral resolution of 0.25 cm^{-1} covering the spectral regime 590-2810 cm^{-1}. As a testbed to the NPOESS candidate instruments, it has been used to simulate "space-like" ground coverage views for the validation of key meteorological species.

5.1.3.2 TES Software Flags and Diagnostics

The processing software will produce error flags and quality metrics at each level that are propagated to the next level either directly or as some average for the level product. An example would be a quality metric for the radiometric calibration based on the number of calibration scans that were averaged and applied. This would be reported for each Level 1B spectrum but could be combined (i.e., averaged) for the Level 2 products which are generated from multiple spectra (usually 64). These combined metrics or other

Level 2 metrics such as the chi-square for the final fit would be mapped by Level 3 to check for orbital and/or regional dependencies. In addition to statistical uncertainties for each profile, Level 2 will also provide average and maximum residual levels, fractions of explained variance (i.e., a measure of the contribution to the retrieval from data compared to *a priori*), correlation distances and total column amounts. Level 2 profiles will also contain an overall quality flag that would be simply good or bad.

5.1.3.3 TES Routine Data Inspection

Diagnostic maps and parameter histories (time series) will be used to monitor instrument and algorithm performance. It will be essential to ascertain very quickly after launch those diagnostic variables that provide the most critical information for visual inspection on a daily basis. While some of the necessary experience regarding instrument health will be obtained pre-launch, the useful set of data quality variables obtained during processing will likely need to be determined from a statistical sample of on-orbit data.

5.1.3.4 TES Radiance Residuals

In order to search for unmodeled species in our data, we will examine the difference between the complete forward model generated from our retrieved atmospheric state and the full TES measured spectrum. Unmodeled species will appear as deviations in the residual that are above the noise level and have characteristic spectral features that can be analyzed using techniques such as Fourier analysis, wavelet transforms or spectral matched filtering. These analyses would be performed on both individual and averaged residuals.

5.1.3.5 Other TES Consistency Checks

Retrievals for species such as H_2O, O_3, CH_4, and N_2O can be performed in many different spectral regions that can be compared for consistency. Since temperature will be retrieved using CO_2 lines, we can perform self-consistency checks by looking for residuals in H_2O and N_2O lines when H_2O is retrieved with the fixed temperature profile retrieved from a previous step. H_2O could have residuals since its absorption features are highly sensitive to temperature variations, while N_2O could be fixed to the relatively well-known abundance to see if the previously retrieved temperatures also fit the N_2O lines. In a later retrieval step, we will retrieve an N_2O profile and use the tropospheric N_2O column as control since a significant deviation from the known column could indicate problems in the other retrieved parameters.

5.1.4 OMI Data Quality Assessment Plans

5.1.4.1 OMI Calibration, Pointing Assessment, and Level 1 Validation

Calibration and pointing

Post-launch activities relating to calibration and pointing are an important part of the data evaluation. These activities include an analysis of engineering data from the instrument, in terms of instrument health and a search for trends in these data (on an orbital or sub-daily bases, as well as on a seasonal, or longer-term basis). The instrument status will therefore be carefully monitored and documented using the engineering and housekeeping data. e.g., the temperature of the CCD detectors will be part of the engineering data and will thus be constantly monitored.

The performance of the OMI-instrument is also verified by performing dedicated measurements during flight, such as White Light Source (WLS) measurements for optical performance of the instrument and for detector characterization, Light Emitting Diode (LED) measurements also for detector characterization, dark-current measurements of the CCD detectors, and sun measurements using different internal diffusers. Furthermore OMI also measures once per day a solar irradiance reference spectrum for a.o. radiometric calibration purposes. The *"In-flight calibration requirements document"* (to be written) describes the use of these dedicated and routinely performed measurements and the engineering data, for instrument health and trend monitoring. Verification of the pointing capability of the OMI-instrument will be done using specific targets, like land-sea boundaries using the small pixel data of the OMI instrument.

OMI Validation of Level 1B Normalized Radiances

The stability of long term observations of OMI data products has high priority, particularly for ozone data. OMI will continue the long-term observations of TOMS ozone column densities and SBUV ozone profiles. Column and profile ozone long-term precision must be on the order of 0.1% and 0.5% per year, respectively. The best way to insure this is to validate Level 1B products in addition to Level 2 products. Level 2 validation provides a check on the performance of the algorithm and does not necessarily need continuous monitoring, although it is desirable for insuring that the algorithms remain applicable under changing calibration and atmospheric conditions..

Cross calibration and validation of OMI Level1B Sun normalized radiances can be accomplished over a broad range of wavelengths in the ultraviolet by means of comparing OMI nadir radiances with zenith sky radiances measured from the ground by a well calibrated spectrometer/radiometer observing over a similar wavelength range. In addition an accurate radiative transfer code that accounts for polarization, multiple scattering, and aerosols is needed to predict the downward and upward radiances.

The technique should be applied to EP TOMS, SBUV/2, SCIAMACHY, QuickTOMS and then to OMI thus insuring continuity of long term ozone trends measured among these instruments. The ground based instrument calibration and corrections to sky radiances due to aerosols and clouds must be precise over the long term to insure that the calibration stability can be tracked with the precision stated above.

Level 1 radiances can also be validated by comparing with other satellite instruments operating in the OMI wavelength range (e.g., GOME and SCIAMACHY). These comparisons may not be independent, but will allow for many cross comparison opportunities and likely reveal systematic biases between measurements. A similar approach was successfully employed in the early GOME validation program.

The solar spectra measured by OMI should be intercompared with spectra measured by other satellite instruments and with published spectra, since inaccuracies in the solar spectra would influence all OMI products, and thus careful checks are very important.

5.1.4.2 OMI Data Quality Controls and Diagnostics

The objective of Data Quality Control is to mark the quality of the data to other users, to indicate where anomalies have been encountered in the data processing and to use quality flags for routine inspection of the instrument performance. The approach the OMI project will take is to perform QA on each level of the data and to automate this process as much as possible. For the Level 1B (Earth radiances, solar irradiances and calibration data) the following QA is planned:

1. incorporate automatic flags for (instrument or software) anomalies in each of the steps in the Level 0 -> 1B processor
2. develop diagnostic tools that perform automated QA on Level 1B data products.

For OMI flags are envisaged for bad engineering data (e.g. too high CCD temperature) but also for bad Level 1B radiance/irradiance measurements caused by bad pixels on the CCD, too high dark current, etc... Plots of radiance/irradiance measurements, dark-current measurements, WLS and LED measurements and time-series of engineering data will be very useful for inspection of the Level 1B data.

For Level 2 and higher data products a similar approach is envisaged and flagging will be used for the Level 2 data products, like ozone column and profile etc..., to indicate specific problems encountered during the Level 1B → 2 retrieval. Simple analyses tools, e.g., for plotting time-series of data and global inspection of the data and flags, will be developed. Estimated uncertainties in the retrieved products will also be a valuable tool for inspection of the data to point out potential problem areas.

Zonal mean maps, daily maps and comparison with climatology data is also envisaged. GOME experience shows that inspection of higher level data (e.g. zonal means, daily maps etc...) can lead to indication of errors in lower level data and can thus be used for routine data inspection.

The OMI QA plans will be described in a separate document.

5.1.4.3 Other OMI Consistency Checks

Another consistency check is to compare different level 2 products that derive the same geophysical quantity. Within the international OMI science team, different methods for the retrieval of ozone column densities, aerosol properties, cloud pressure and cloud fraction are being developed. The results of these methods will be critically evaluated through intercomparisons.

5.2 Aura Geophysical Data Validation: Needs, Priorities, and Plans

The goals of this section are the following: to review the framework for validation of geophysical data; to present a table of sources of correlative data that are expected during the few years after the Aura launch; to discuss requirements for space and time coincidence for correlative data; to discuss the desired spatial and temporal coverage for various validation studies; and to focus on the type, timing, and desirability of specific campaigns (aircraft and balloon flights in particular) that address both validation and scientific issues relevant to Aura. Major campaigns require about two years of advance planning.

5.2.1 A Framework for Validation of Geophysical Data

The various aspects of validation studies relating to intercomparisons of geophysical data are summarized by the schematic further below. The term “core validation phase” includes the “instrument activation phase” and the “commissioning phase.” The “long-term validation phase” refers to the time from the end of core validation (about 3 years from launch) to the end of mission, although in practice, there may be some overlap between core validation and long-term studies.

Instrument activation includes degassing and initial checkout, and should be completed for all instruments within the first three months of Aura deployment. TES anticipates three months to accommodate degassing, while MLS may begin to acquire data in a near-routine mode about one month after the satellite has reached its desired stable orbit.

Preliminary assessment of Aura products will take place during the following six months, the commissioning phase. Internal consistency checks and validation studies for at least the main products will take place during this time period. Comparisons against climatological or model values will be part of this first-order sanity check of the retrievals. Stratospheric profiles will be examined for problems first in the mid-stratosphere and upper stratosphere, where contributions from water vapor, aerosols, clouds, and contaminating gases are minimal. Tropospheric products from unpolluted regions with small albedo variations (i.e., over the ocean) and under moderate solar zenith angles will be examined first. Some intercomparisons among Aura instruments will be performed, along with a few correlative studies on a global basis to check for spatial differences using validated satellite-based measurements and some assimilated satellite data. Uncertainty estimates will be evaluated, with a focus on random errors (precision), based on empirical repeatability during quiescent conditions. Some first-order biases (systematic errors) will probably emerge. A validation workshop is expected after this phase is completed, for Aura-wide discussion and summary of these early results (Table 5.1).

The remainder of the core validation phase will include more difficult retrievals, including the lowermost altitude ranges for profiles, polluted tropospheric conditions, etc...) and utilize correlative data from various sources, including major campaigns (indicated with large symbols on the chart). Small campaigns at fairly regular intervals (e.g., balloon launches at equinox, or similar activities) would also take place during this phase; routine measurements (e.g., ozonesondes, radiosondes) will take place more frequently (weekly or even daily). We envision that the first major aircraft/balloon campaign would be scheduled to take place about 1 year after launch. Such a schedule could accommodate a delay in the Aura launch and would still take place well after instrument activation. Core validation will be completed by about the third year after launch, with much of the final year needed for summary analyses and write-ups. If a better final data set is developed later, many of the intercomparisons would be repeated using that data set. A tentative top-level schedule for validation workshops is given in Table 5.1. This schedule includes pre-launch activities such as a validation rehearsal to test accessibility to validation data sets and to exercise some of the software to be used during the post-launch comparisons. Plans must be made for the storage of correlative data, particularly from ground-based networks, and to enable exchange of data among Aura data providers and correlative investigators (section 6).

The “long-term validation phase” will encompass any further validation studies and will utilize as much correlative data as possible. It will include data products that are more difficult to retrieve or validate, as well as validation of observed longer-term variations and trends. The latter studies will address instrument stability and degradation issues. Data produced during Aura reprocessing in this later phase will necessitate additional validation. Refinements in uncertainty estimates will be made during this phase.

Validation Methods

Satellite-based atmospheric observations require high precision and stability over long time periods, in addition to high accuracy; offsets related to inaccuracies (systematic errors) are often viewed as less critical than stability over time, which is crucial for defining atmospheric/climate changes ranging from percents per year to less than a percent per decade. Ground-based networks, in conjunction with other satellite measurements, can provide the validated data sets that are needed for studying such changes.

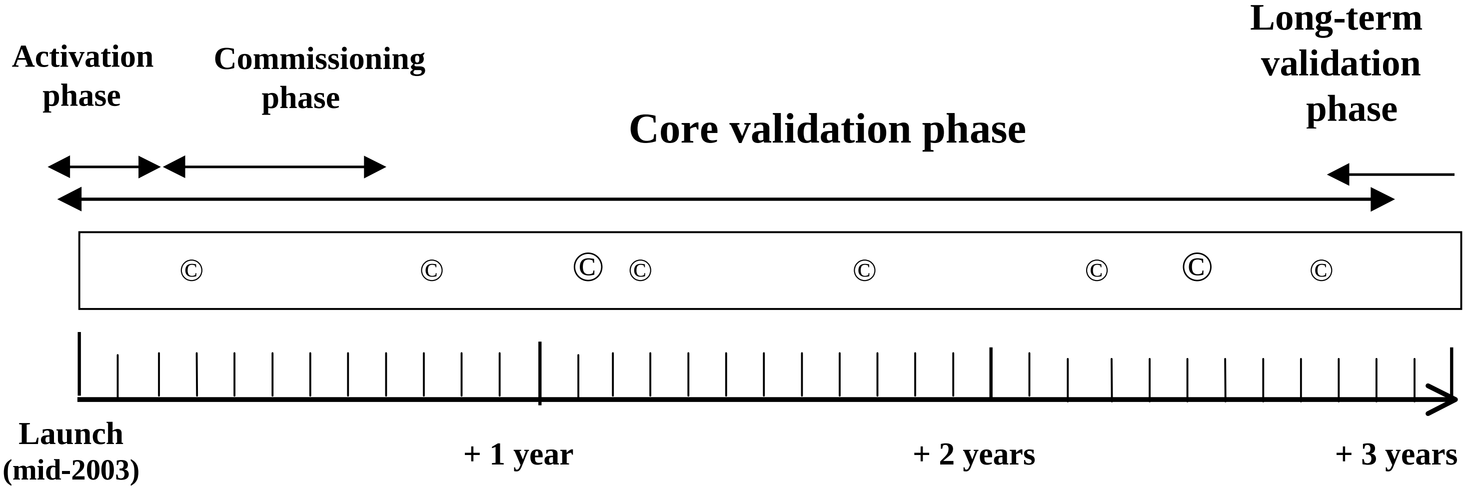
If there are disagreements in the ensuing intercomparisons, past experience shows that the reasons will usually differ from dataset to dataset. Most of the broad reasons for disagreements include one or more of the following: poor calibration or poor calibration stability (in one or both of the datasets being compared), poor error assessment (often too conservative), inaccurate retrievals (transformation from raw measurements to geophysical product), poor match between measurements (e.g., sampling issues, or resolution issues), or actual atmospheric variability (although this source of error should be removable given enough statistics for comparison).

There is no recipe for predicting or solving discrepancies that may arise in the future, apart from careful planning for all of the aspects mentioned in this document in relation to calibration and validation (this is true, of course, for both satellite and ground-based systems). Each instrument has (had) its own observing characteristics, advantages, and disadvantages. Past experiences and published validation papers (e.g., JGR special issue, April 30, 1996, “Evaluation of the UARS Data”, WMO/SPARC Report, 1998) should serve as a guide. “Lessons learned” include avoiding premature scientific publications before high enough confidence in the data sets exists (although this has to be balanced with a need to disseminate solid new information).

One of the issues Aura will have to face (more so than UARS) is one of validation between coarse sampling in the troposphere and lower stratosphere, where spatial and temporal atmospheric variability can be large, and significantly different sampling systems for correlative studies (e.g., from balloons or aircraft). This is discussed at some more length in section 5.2.3.1.3, but it is fairly uncharted territory. Validation of UARS MLS upper tropospheric water vapor profiles (Read et al., 2001) is a recent example where sufficient correlative radiosonde data exist (but this is not true for most other constituents in the troposphere). Validation of MOPITT measurements of tropospheric CO and CH_4 column densities is an example still in its early stages, where fine scale profiles obtained from aircraft are being used to produce simulated radiances for comparison with the spaceborne radiance measurements (as one step in the validation process). Comparisons of profiles with significantly different vertical resolution should entail averaging of the fine resolution profiles (using averaging kernel information for the satellite-based retrieval system). Moreover, the use of correlative data is evolving from the simple comparisons of “coincident data” to methods involving more complex mapping between measured products, in order to provide more robust statistics (e.g., through the use of trajectory calculations to match a larger number of “coincident” air parcels). For Aura validation studies, we advocate comparisons of geophysical measurements obtained through independent and different techniques (if possible), with an emphasis on building statistics through traditional coincident measurements enhanced by other modeling, mapping, and assimilation efforts (see section 5.2.5).

A Framework for Validation of EOS Aura

- **Schematic of timeline for validation**



© = major validation campaign, © = minor validation campaign (schematic timeline)

- **Correlative data needs are driven by a desire for sufficient statistics and for comparisons under differing atmospheric and viewing conditions**

- **Some desirable attributes of correlative data**
  - **Accuracy:** well-validated measurements are needed for validation of Aura data products
  - **Temporal coverage:** e.g., comparisons from fixed sites (for seasonal and longer-term studies)
  - **Spatial coverage:** various latitudes/regions offer different atmospheric conditions for comparison

    Examples of useful conditions (a) tropics (dry season)
    (b) polar vortex (winter/spring)
    Having both of the above provides a check on both high and low tropopause conditions
  - **Scientific value:** valuable scientific goals are defined for the correlative data set or mission
  - **Further points:**

    - **Profiles** are needed (often from ground to upper strat.) + column data (mainly for OMI & TES
    - Some averaging (spatial/temporal) of Aura profiles will sometimes be required for comparison
    - Atmospheric variability is an issue for coincidence criteria, especially in the troposphere
    - Ideally, would like to have 2 (or more) correlative data sets or techniques for comparison
    - Photochemical models, data assimilation, and other methods can enhance validation studies

- **A variety of correlative data sources will be needed and used**

  A. Fixed sites (balloons, sondes, NDSC data, Dobson network, ARM data, ...)
  B. Campaigns (aircraft/balloon missions; profiles along Aura measurement tracks are desirable)
  C. Global data sets (other satellite data, operational meteorological data, ...)

Table 5.1. Top level schedule of plans for the main Aura validation activities (not including the long-term validation phase). The "L ± nm" notation refers to the Aura launch date ± "n" months.

Aura
Launch
⇓

3 years before launch	**2 years before launch**	**1 year before launch**	**1 year after launch**	**2 years after launch**	**3 years after launch**
Pre-launch Phase			**Core Validation Phase**		
Build, calibrate, integrate instruments			Post-launch calibration		
Produce launch-ready retrieval software (simulations, error analyses)			Improve upon retrieval algorithms; characterize errors.		
Improve upon spectroscopic database					
Gather and analyze "instrument-type" data (radiances) + other databases					
Produce Validation Plan	Make Specific Validation Plans (+ review/select proposed validation studies)		Coordinate, gather, & analyze correlative data (for comparison with Aura data)		
	Form Validation Teams		**L to L+3m:** Instrument activation phase **L+4m:** Preliminary assessment of initial results **L+9m:** Workshop: Intercomparisons, and results from first 3 to 6 months of data and "campaigns"	**L+18m:** Workshop: results from first 12-15 months of data & campaigns	**L+27m:** Workshop: results from first 21-24 months of data and campaigns
		Select correlative data formats, data archival & transfer methods. Implement and rehearse.			

5.2.2 Correlative Data Sources

5.2.2.1 Ground Networks

Brief summary information about ground networks is provided below. More information about data access issues will be addressed in a later update of this document.

NDSC (Network for Detection of Stratospheric Change): A map for this network is provided in Fig. 5.1**.** This network includes ~60 ground-based stations worldwide and a few mobile instruments, aimed at high-quality remote sensing of stratospheric composition and its changes over time.
Sites: There are 5 primary stations with a number of sites: Arctic station (Eureka, Canada; Ny Alesund, Norway, Thule, Greenland; Sondre Stromfjord, Greenland); "Alpine" station (Garmisch, Germany; Zugspitze, Germany; Bern, Switzerland; JungfrauJoch, Switzerland; Observatoire de Bordeaux, France; Plateau de Bure, France; Observatoire de Haute Provence, France); Hawaii station (Mauna Kea, U.S.A; Mauna Loa, U.S.A., Hilo, U.S.A.); New Zealand station (Lauder), Antarctic station (Dumont d'Urville, McMurdo, Arrival Heights, Scott Base, South Pole). There are also about 40 complementary sites/stations (only a few in the tropics). A few instruments (ozone/temperature lidar, aerosol/temperature lidar, microwave, FTIR) can be moved for campaign purposes.
Instruments and products: ozonesondes (O_3 profiles), Dobson instruments (O_3 columns), lidars (T, O_3, and aerosol profiles), microwave instruments (O_3, ClO, H_2O, N_2O profiles), Fourier transform infrared spectrometers (many different column measurements, including O_3, CH_4, N_2O, HNO_3, CO, NO, NO_2, $ClONO_2$, HCl, HF, CH_2O, and some profile information), UV/VIS instruments (column NO_2, O_3, OClO, BrO), aerosol sondes (aerosol backscatter profiles), and spectral UV instruments (spectral distribution of UV irradiance at the ground).
Reference: http://www.ndsc.ws

ARM (Atmospheric Radiation Measurement) Program: Initiated by the U.S. Department of Energy in 1989, with 3 highly instrumented facilities (Climate and Radiation Test Beds, or CART) to measure the radiative energy flux profile of the clear and cloudy atmosphere.
Sites: 3 main sites (Southern Great Plains site in Oklahoma, Alaska site, Tropical Western Pacific site).
Instruments and products: Combined data from microwave, infrared, lidar, and sonde instruments for near-continuous profiles of T and H_2O in the troposphere; some aerosol information from Raman lidar.
Reference: http://www.arm.gov/

AERONET: This Aerosol Robotic Network is a ground-based network (with over 60 sites) of sun photometers for the derivation of aerosol parameters [Holben et al., 1998; see also http://aeronet.gsfc.nasa.gov:8080/].
Aerosol Database:
WMO-related database, located in Ispra, Italy.

COSE (Compilation of atmospheric Observations in support of Satellite measurements over Europe):
European database of many different species, including ozone profiles, ClO, BrO. Supported by the European Union (until date to be determined).
Reference:http://www.nilu.no/projects/nadir/cose/cose.html

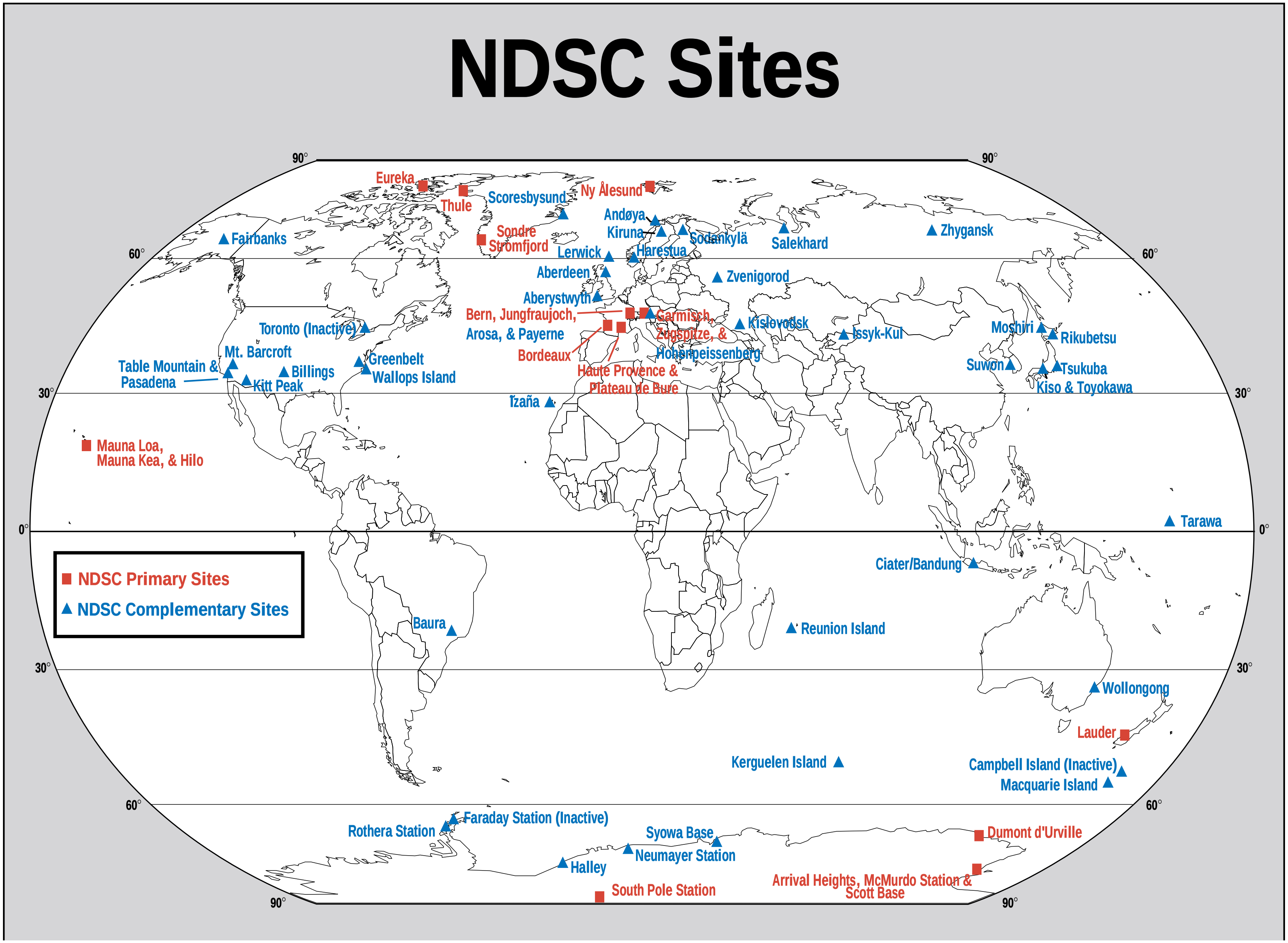


Figure 5.1. Map of NDSC site locations (provided by M. Kurylo).

Radiosonde Network: Over 1300 radiosonde sites exist worldwide for T and H_2O profile measurements, obtained typically once or twice per day, mainly in the troposphere (especially for H_2O). Wind is also measured (rawinsonde term is also used). A map of the sonde data locations archived by NOAA's National Climatic Data Centers Comprehensive Reference Data Sets is shown in Figure 5.2 below.

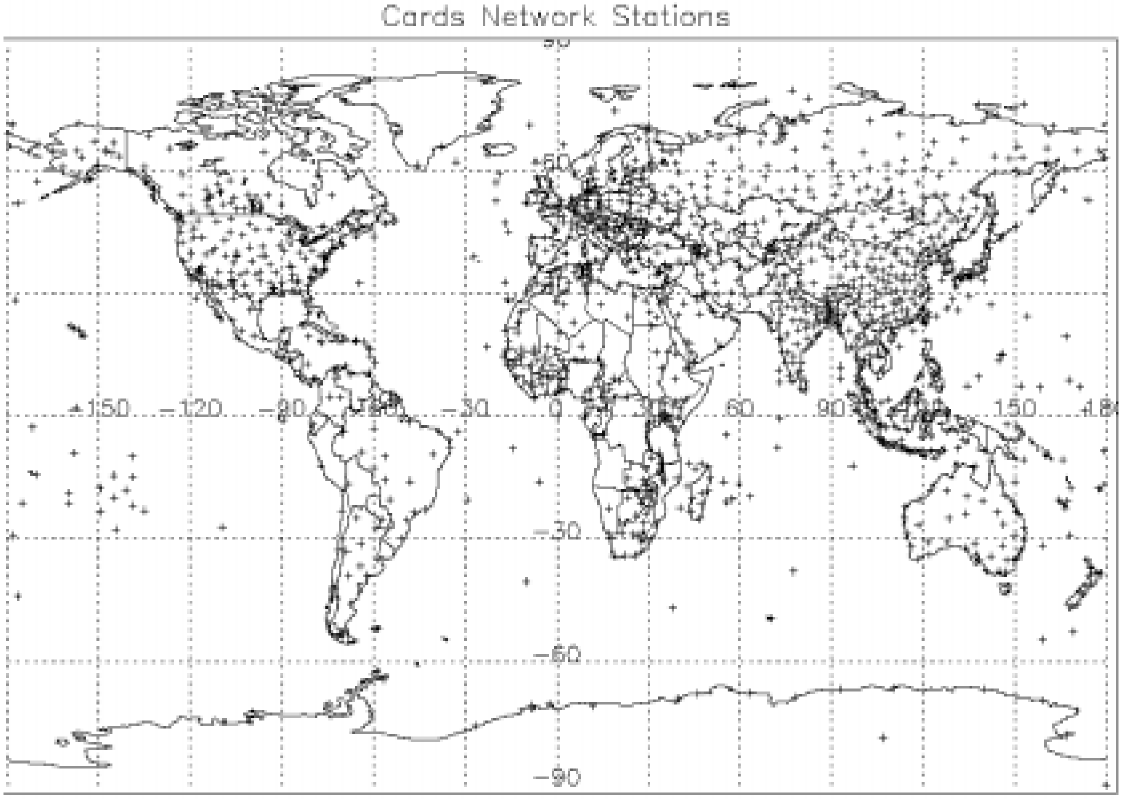


Fig. 5.2. CARDS Network of meteorological sonde sites.

WOUDC (World Ozone and UV Data Center – WODC and WUDC) and SHADOZ:

WODC and SHADOZ:

The Toronto World Ozone Data Center (WODC) (under WMO and operated by the Meteorological Service of Canada) contains extensive archives of ozone profile and ozone column data. Sondes for ozone (and T, usually) are launched from 50 to 100 sites around the world, about once a week (some less often, some more often). The altitude range is typically from the ground to about 30 km. A recent program called SHADOZ (Southern Hemisphere Additional Ozonesondes) has provided measurements from 10 locations in the southern tropics and subtropics during the period 1998-2000.

References: http://www.t or.ec.gc.ca/woudc/,
http://code916.gsfc.nasa.gov/Data_services/shadoz

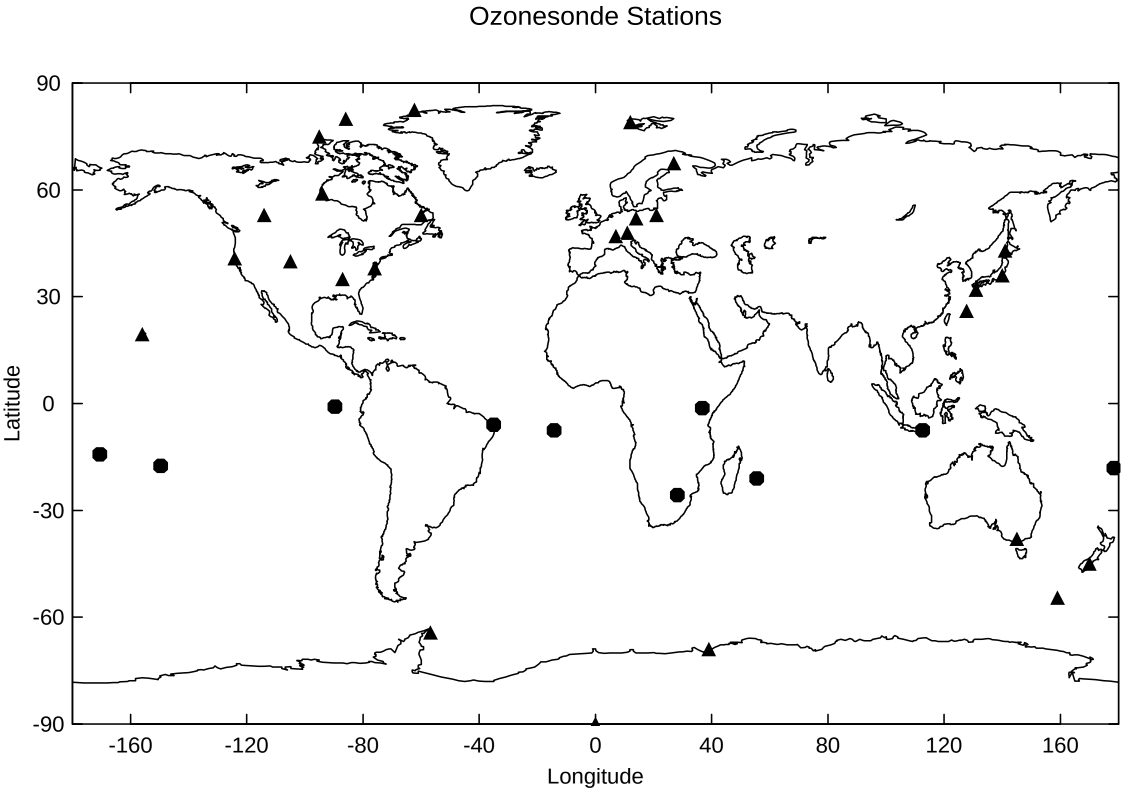


Fig. 5.3. Ozonesonde stations reporting data in 1998 and/or 1999. SHADOZ data (filled circles above) are available from the SHADOZ website, and other data (triangles) from WODC, CMDL, and other sources.

WUDC: (World Ultraviolet Data Center)

Contains, as above, extensive archives on ultraviolet data.

Reference: http://www.tor.ec.gc.ca/woudc/

Other Networks

Other networks and databases exist, such as the Brewer-Dobson and Umkehr ozone networks, and the column measurements from the SAOZ (Système d’Analyse par Observation Zénithale).

5.2.2.2 Satellite Data

Table 5.2. Satellite instruments planned during the 2000-2008 time period, along with Aura. Satellite names are followed by instrument names, with those thought to be of most relevance to the Aura validation plans indicated in bold. Solid diamonds indicate launch date (or expected launch date), and arrows give approximate date for nominal end of mission, beyond which more data can often be expected. See Appendix B for more details/references.

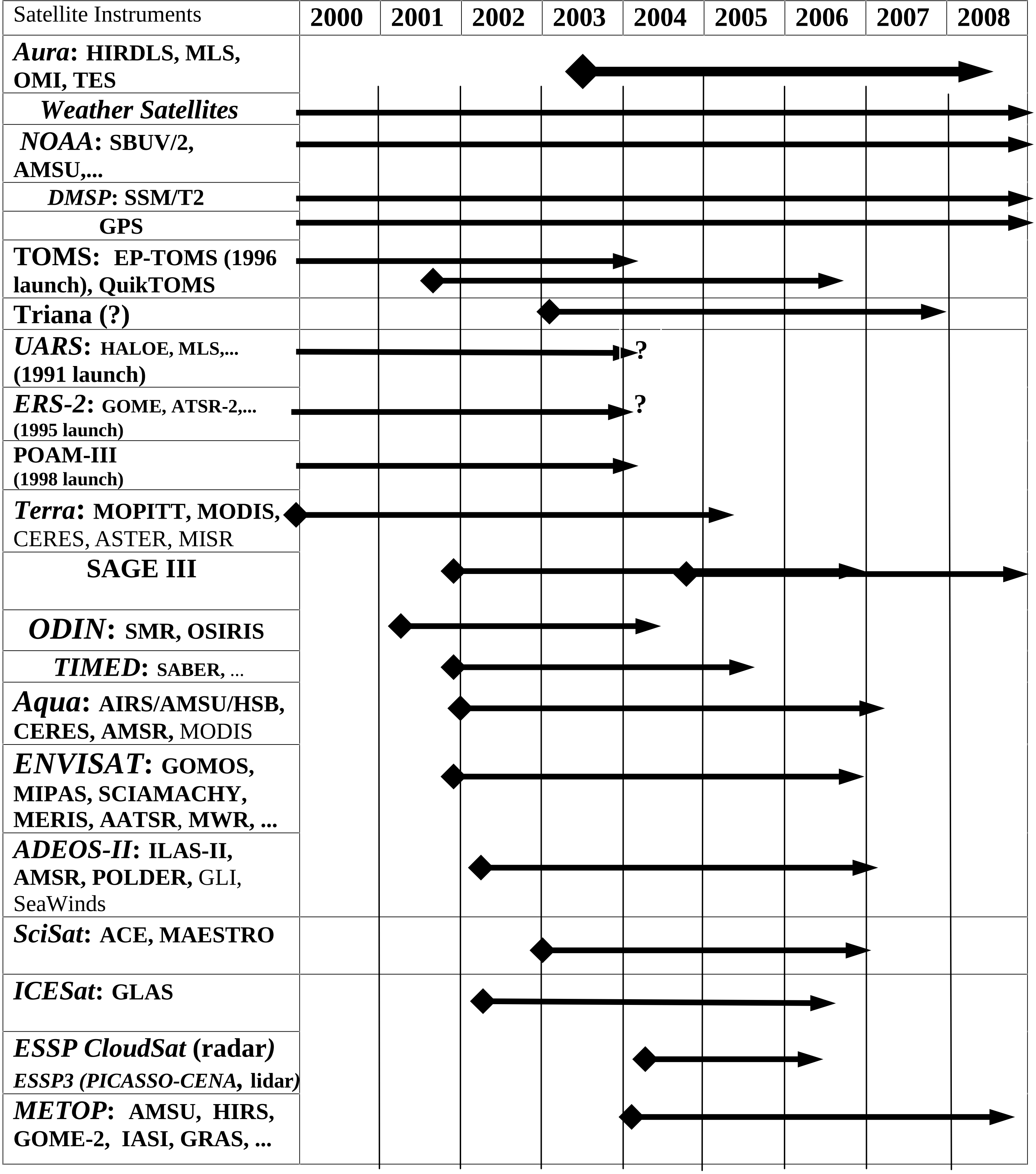


Table 5.2 summarizes anticipated satellite data sets most relevant to the Aura measurements, during the 2000 to 2008 time period, along with expected lifetimes. Some, such as UARS, have question marks as they are past their design lifetime and may not survive until Aura launch.

There are synergistic possibilities for intercomparisons (and science/validation goals) among the measurements obtained by the Aqua, Aura, and the ESSP CloudSat and ESSP3 (formerly PICASSO-CENA) missions, since the polar orbits for these missions will be very similar: the (ascending) equatorial crossing time for Aqua (at 1:30 p.m.) is 15 minutes ahead of that of Aura (1:45 p.m.). If Aura also flies 15 minutes later along its orbit (i.e. following Aqua), the ground tracks should be basically coincident. Flying Aura 7 minutes later along the Aqua orbit would allow MLS views (ahead of Aura by that amount) to match the Aqua ground tracks; TES nadir views and HIRDLS views could be adjusted (to the "side") in order to also match the Aqua ground tracks. CloudSat and ESSP3 (PICASSO-CENA) should fly only 1 minute later than Aqua, so that good coincidence possibilities will also be quite possible with this mission. ENVISAT has a 10 a.m. descending equatorial crossing time (similar to Terra's 10:30 a.m. descending crossing time), which is not conducive to tight temporal coincidences with most Aura measurements.

5.2.2.3 Aircraft and Balloon Data

Measurements of temperature, constituents, aerosols and clouds are possible from aircraft both in the troposphere (e.g., U.S. DC-8, altitudes up to about 10 km) and in the lower stratosphere (e.g., U.S., ER-2, altitudes up to about 21 km). In situ measurements are made at the aircraft cruise altitude. Measurements from lidar and microwave instruments provide profiles of ozone and temperature above and below the DC-8. A small number of profiles of temperature and constituents can be made when the aircraft ascends and descends during takeoff and landing, or during a dive maneuver using in situ instruments.

The constituents observed by Aura can be measured using balloon-borne instruments; these may be in situ or remote sensing devices. Balloon profiles are essential for stratospheric comparisons up to about 40 km.

Most aircraft and balloon data sets will be made in "campaign mode" after the first year of Aura measurements, however a series of regular balloon flights during the years following launch is needed. The need for regular data sets and the need for frequent observations in the troposphere is discussed in section 5.2.3.5.

5.2.2.4 Summary of Potential Correlative Data Sources

Table 5.3 lists the main products for which profiles are expected from Aura and identifies both routinely available data sets (as from the Dobson network or the Network for Detection of Stratospheric Change (NDSC)) and "campaign-type" data sets, primarily from aircraft and balloons. Some data sets included as "routine mode" could also be used as part of a campaign (e.g., for better timing of coincidences with Aura overpasses) but these are not duplicated in the table. Examination of entries in this table shows that routine measurements will not meet the need for correlative observations for all of the Aura products. Needs and priorities are discussed below (section 5.2.3.2)

Table 5.3. Potential Correlative Data Sources for EOS Aura Measurements. This Table lists the EOS Aura data products and potential correlative data sources, as a function of altitude. Data sources are classified into broad categories for “campaign mode” and “routine mode”, although some measurements from the latter category might also be geared specifically to optimize certain campaign mode requirements. The measurement techniques are distinguished by the following general types: OM-data (Operational Meteorological data), A (Aircraft), B (Balloon), sonde (or small balloon), rocket, G (Ground-based), or by the satellite acronyms. Measurement techniques (for A, B, or G types) are broadly defined by the following abbreviations: IR (infrared techniques, e.g. occultation, or emission), MW (microwave, or near-millimeter wavelengths), lidar, UV (ultraviolet), VIS (visible), in situ (for in situ measurements), and data (for both in situ & remote sensing techniques).

TH stands for tropopause height. Altitude range is meant to be approximate, with typical ranges of “TH-4 to TH” representing the upper troposphere, “TH to 20” representing the lower stratosphere (accessible by airplanes for correlative data sources), “20 to 40” representing the middle stratosphere (accessible by balloons and in part by sondes/small balloons), and “> 40” representing the upper stratosphere and mesosphere (and above), which are generally not accessible by balloons.

Aura instruments providing the measurements are indicated by H (HIRDLS), M (MLS), O (OMI), and T (TES).

Geophysical Parameter	**Altitude range (km)**	**Aura instrument**	**Potential Correlative Data Sources**	
			“Campaign” mode	**“Routine” mode**
Temperature	0 to TH-4	T	A-data, Radiosonde	Radiosonde, OM-data, G-lidar, ARM, GPS, AIRS, AMSU, SCIAMACHY
	TH-4 to 30	H, M, T	A-data, Radiosonde	Radiosonde, OM-data, G-lidar, ARM, UARS?, POAM III, ACE, GPS,SABER,AIRS, AMSU, MIPAS, SCIAMACHY, ILAS-II
	30 to 40	H, M, T	B-data	OM-data, G-lidar, GPS, SABER, UARS?, POAM III, ACE, AIRS, GOMOS, MIPAS, SCIAMACHY, ILAS-II
	40 to 60	H, M	Rocket	G-lidar, rocket, UARS?, GPS, SABER, AIRS, GOMOS, MIPAS, SCIAMACHY, ILAS-II
Geopotential Height	TH to 60	H, M	Radiosonde	OM-data, GPS
BrO	20 to 40	M$^{(**)}$	B-in situ	SCIAMACHY, GOMOS (during enhanced polar / ozone hole conditions)
BrO Column	Total Column	O, (M$^{(**)}$)	B-UV/VIS	G-UV/VIS, GOME, SCIAMACHY
CFC-11,CFC-12	TH to 20	H	A-in situ, B-data	MIPAS, ILAS-II, ACE
	20 to 27	H	B-data	
CH_3CN	TH to 40	M$^{(*)}$	A-in situ, B-in situ	MIPAS, ILAS-II, ACE
CH_4	0 to TH	T	A-in situ, B-in situ	Surface stations, MOPITT (column)
	TH to 20	H, T	A-data, B-data	HALOE?, MIPAS, SCIAMACHY, ILAS-II, ACE
	20 to 40	H, T	B-data	HALOE?, MIPAS, SCIAMACHY, ILAS-II, ACE
	> 40	H		HALOE?, MIPAS, ILAS-II, ACE

ClO	TH to 20	$M^{(*)}$	A-in situ, B-data	G-MW, UARS MLS ?, ODIN
	20 to 40	$M^{(*)}$	B-data	G-MW, UARS MLS ?, ODIN, SCIAMACHY (during enhanced polar conditions)
	> 40	$M^{(**)}$	B-data	G-MW, UARS MLS ?, ODIN
$ClONO_2$	20 to 35	H	B-IR	MIPAS, ILAS-II, ACE
CO	0 to TH-4	T	A-in situ, B-in situ	G-IR (total column)?, A-MOZAIC, MOPITT
	TH-4 to TH	$M^{(*)}$, T	A-in situ, B-in situ	A-MOZAIC, MOPITT, MIPAS(?)
	TH to 20	$M^{(*)}$, T	A-in situ, B-data	A-MOZAIC, MOPITT, MIPAS, SCIAMACHY, ACE
	20 to 40	$M^{(*)}$, T	B-data	ODIN, MIPAS, SCIAMACHY, ACE
	> 40	$M^{(*)}$	Rocket	ODIN, MIPAS, SCIAMACHY, ACE
HCHO Column	Total Column	O	G-UV, A-in situ	GOME? SCIAMACHY, (ACE)
HCl	TH to 20	M	A-in situ, B-IR	HALOE?, ACE, G-IR (total column)
	20 to 40	M	B-IR	HALOE?, ACE
	> 40	M		HALOE?, ACE
HCN	TH-4 to 20	M	B-data	(G-MW), ACE
	20 to 40	$M^{(*)}$	B-data	G-MW, ACE
	> 40	$M^{(**)}$		G-MW, ACE
HNO_3	0 to TH	T	A-in situ	G-IR (total column)?
	TH to 20	H, $M^{(*)}$, T	A-data, B-data	G-MW, (G-IR), UARS MLS?, ODIN, MIPAS, ILAS-II, ACE
	20 to 40	H, $M^{(*)}$, T	A-IR, B-data	G-MW, (G-IR), UARS MLS?, ODIN, MIPAS, ILAS-II, ACE
	> 40	$M^{(**)}$		G-MW, ODIN, ACE
HOCl	20 to 40	$M^{(**)}$	B-IR	ACE
HO_2	20 to 40	$M^{(**)}$	A-in situ, B-MW, B-IR	ODIN
	> 40	$M^{(**)}$		ODIN

H_2O	0 to TH-4	T	Radiosonde, A-data, B-data	Radiosonde, OM-data, A-MOZAIC, G-lidar, UARS? , SAGE, ARM, GPS, AIRS, AMSU, SCIAMACHY, AMSR, SSM/T2, Weather satellites
	TH-4 to TH	H, M, T	Radiosonde, A-data, B-data	Radiosonde, OM-data, A-MOZAIC, G-lidar, UARS?, SAGE, ARM, GPS, AIRS, AMSU, MIPAS, SCIAMACHY, AMSR, SSM/T2, Weather satellites
	TH to 20	H, M, T	A-data, B-data	UARS?, SAGE, POAM III, ODIN, SABER, GOMOS, MIPAS, SCIAMACHY,ILAS-II, ACE
	20 to 40	H, M, T	B-data	G-MW, UARS?, SAGE, POAM III, ODIN, SABER, MIPAS, SCIAMACHY, ILAS-II, ACE
	> 40	H, M		G-MW, UARS?, SAGE, POAM III, ODIN, SABER, MIPAS, SCIAMACHY,ILAS-II, ACE
NO	0 to TH-4	T	A-in situ, B-in situ	G-IR (column)?
	TH-4 to TH	T	A-in situ, B-in situ	?
	TH to 20	T	A-in situ, B-data	HALOE?, ACE
	20 to 40	T	B-data	HALOE?, ACE, MIPAS (and ODIN, SCIAMACHY for > 40 or 50 km)
NO_2	0 to TH-4	T	A-in situ	G-IR (column)?, SCIAMACHY
	TH-4 to TH	T	A-in situ	SCIAMACHY, MIPAS?
	TH to 20	H, T	A-in situ, B-IR	HALOE?, SAGE, POAM III, ODIN, GOMOS, MIPAS, SCIAMACHY, ILAS-II, ACE
	20 to 40	H, T	B-IR	HALOE?, SAGE, POAM III, ODIN, GOMOS, MIPAS, SCIAMACHY, ILAS-II, ACE
NO_2 Column	Total Column	O	A-UV/VIS, B-UV/VIS	G-VIS, GOME, HALOE?, SCIAMACHY
NO_2 Column (tropospheric)	Trop. Column	O, O-H, O-T	G-lidar, A-UV/VIS, B-UV/VIS, G-VIS	G-VIS, GOME, SCIAMACHY, G-in situ (SOS, etc...) combined with meteorological models
N_2O	0 to TH	T	A-in situ	SCIAMACHY
	TH to 40	H, M, T	A-data, B-data	G-MW, ODIN, MIPAS, ILAS-II, ACE
	> 40	H, M	Rocket	G-MW, ODIN, MIPAS, ILAS-II, ACE
N_2O_5	TH to 45	H	B-IR	MIPAS, ACE
OClO Column	Total Column	O	B-UV/VIS	G-UV/VIS, GOME, SCIAMACHY

OH	20 to 30	$M^{(**)}$	A-in situ, B-data	G-UV (Total Column)
	30 to 40	$M^{(*)}$	B-data	
	40 to 60	M		
O_3	0 to TH-4	O, T	A-data, B-in situ, sonde	Sonde, G-lidar, A-MOZAIC
	TH-4 to TH	H, $M^{(*)}$, O, T	A-data, B-in situ, sonde	Sonde, G-lidar, A-MOZAIC
	TH to 20	H, M, O, T	A-data, B-data, sonde, G-lidar	Sonde, G-lidar, UARS?, GOME, SAGE, ODIN, SABER, MIPAS, SCIAMACHY, ILAS-II, ACE
	20 to 40	H, M, O, T	B-data, sonde, G-lidar	Sonde, G-lidar, G-MW, G-SAOZ, Umkehr, UARS?, GOME, SAGE, POAM III, ODIN, SABER, GOMOS, MIPAS, SCIAMACHY, ILAS-II, ACE
	> 40	H, M, O	G-lidar	G-lidar, G-MW, Umkehr, UARS?, GOME, SAGE, ODIN, SABER, GOMOS, MIPAS, ILAS-II, ACE
O_3 Column	Total Column	O		Brewer, Dobson, Umkehr, G-UV/VIS, sonde, G-lidar, TOMS, GOME, AIRS, SCIAMACHY
	Trop. Column	T,O,O-H, O-M	A-UV/VIS	Profiling instruments (e.g., sonde, G-trop. lidar), GOME, TOMS
	Strat. Column	H, M, O	A-UV/VIS	Profiling instruments (e.g., sonde, G-strat. lidar, G-MW)
SO_2 (volcanic)	TH to 20	$M^{(*)}$	A-in situ, B-IR	SCIAMACHY, ACE
	20 to 40	$M^{(*)}$	B-IR	SCIAMACHY, ACE
SO_2 Column (volcanic)	Total Column (volcanic)	O, T, (M)	A-COSPEC, B-Brewer	G-UV/VIS, G-Brewer, COSPEC, SCIAMACHY, TOMS (Column), GOME
SO_2 Column (background)	Total Column (background)	O, T, (M)		Under background conditions, low Aura sensitivity to SO_2, and no strong need for validation.
Aerosol opt. thickness		O	A-data, B-in situ	G-lidar, G-photometer, SAGE, GOME, TOMS, POLDER, SCIAMACHY
Aerosol single scatt. Albedo		O	A-data, B-in situ	G-lidar, G-photometer, SAGE, GOME, TOMS, POLDER, SCIAMACHY
Aerosol Opacity	TH-4 to 20	H, T	A-data, B-in situ	G-lidar, G-photometer, SAGE, POAM III, GOME, POLDER, SCIAMACHY, ILAS-II

Cloud Ice (upper trop.)	TH-4 to TH	M	A-data	CloudSat, AIRS, (MODIS), (MERIS)
Cloud Fraction[a]		H, O, T	A-data, B-data	WMO Network ?, ARM?, Weather satellites, ATSR-2, GOME, AIRS, MODIS, CloudSat, ESSP3(PICASSO-CENA)
Cloud Height or Pressure[a]		H, O, T	A-data, B-data	G-radar, ARM?, Weather satellites, ATSR-2, GOME, ODIN, AIRS, MODIS, ENVISAT, ILAS-II, CloudSat, ESSP3(PICASSO-CENA)
PSC	TH to 20	H, T	A-data, B-in situ	G-lidar, SAGE, ESSP3(PICASSO-CENA)
UV spectra & UV-B flux		O	UV spectrometers	G-UV, TOMS
Upwelling radiance (650-3050 cm^{-1})		T	A-data, B-data	MODIS?, ASTER?

(*) Measurements will often require some averaging

(**) Measurements will always require some averaging

[a] Note that cloud fraction and pressure will have different interpretations among the instruments (and wavelength dependence exists)

SAGE, above, refers to data from SAGE III (and SAGE II, if available).

GOME, above, refers to data from GOME and/or GOME 2 (GOME 2 only for long-term validation, since launch is planned for 2005)

5.2.3 Validation Priorities and Approach

We expect to use correlative data sets from the full range of available platforms (ground, balloon, aircraft, and satellite data).

During the commissioning phase, intercomparisons will be made among products that are common to more than one instrument from Aura (see section 3.1). These will include comparisons of series of near-coincident profiles along the satellite track. For some Aura measurements comparisons may be made with previously validated observations from satellite or ground based instruments. Initial validation efforts will focus on measurements made under optimal conditions for which the algorithms are expected to work relatively well. For OMI, this means moderate zenith angles and cloud-free regions (or pixels); data would be compared with that from a similar nadir-viewing satellite instrument (such as SCIAMACHY) and with data from ground-based instruments. Retrievals of stratospheric profiles tend to increase in difficulty as the altitude decreases towards the tropopause, as constituent mixing ratios often decrease and there is more contamination from H_2O, aerosols, and clouds.

The profiles obtained regularly from a set of sites will play an important role in the core validation phase, especially for some Aura products that are not easily measured from other platforms. It is obvious that contemporaneous measurements from instruments on other satellites (e.g., SCIAMACHY on ENVISAT) are faced with similar validation challenges. This data comparison period should continue for about two years, starting a few months after launch, and could involve a variety of sources (from daily or weekly profiles for certain networks to large balloon flights twice or more per year).

For most (if not all) stratospheric profiles, validation studies will **not** depend primarily on one or two specific aircraft campaigns. Significant use will be made of well-calibrated, validated profiles taken “routinely” at a variety of times and locations, as was done for the validation of Upper Atmosphere Research Satellite data. Correlative data used in validation was mainly fairly regular data sets (see special issue of *J. Geophys. Res.*, Vol. 101, No. D6, April 30, 1996). The ground and satellite networks described above provide a good database for comparison with a significant number of Aura measurements, as long as sufficient validation of these data has been performed prior to Aura launch. A minimum of a year is generally required to produce and validate high quality data sets from satellite observations. The need to reprocess the data can delay the availability of the validated data. Areas where more correlative data would be desirable are mentioned below.

Aircraft data will be essential for validation of tropospheric profiles and tropospheric column densities. Ozone is the only species for which regular profile measurements are made. The requirements for temporal and spatial coincidences in the troposphere will be more stringent than for the stratosphere, because of high variability in many regions. There are however regions/seasons with smaller variability (e.g., the southern mid-Pacific in March/April). One or two aircraft campaigns will provide essential but insufficient data for validation. For example, during the TRACE-P mission in spring 2001, validation profiles were obtained for a single overpass of Terra on half of the flights in the second part of the campaign. For a typical tropospheric campaign of about 20 8-hour flights, validation profiles would be obtained for only about 10-15 overpasses, allowing for cloudiness. Most campaigns focus on a fairly large region, but they do not generally cover both the mid-latitudes and tropics. An absolute minimum requirement would be for a mid-latitude and a tropical aircraft campaign, to provide data for the range of conditions typically encountered in the troposphere. Any tropical campaign would require data above the ceiling of conventional aircraft, about 12 km. Campaign aircraft data will have to be supplemented by other profile measurements. These could be provided by aircraft equipped with instrumentation that is focussed on validation needs. This is discussed further in the following section. Validation of MOPITT on Terra includes bimonthly flights of sampling equipment on chartered aircraft that reach 7-8 km from 5 sites. A similar program with an aircraft that reaches higher altitudes may be required for TES validation and OMI tropospheric column validation.

An attempt is made in section 5.2.3.2 to establish priorities for the various products from within each of the Aura instruments' suite of measurements. The overall goal is to validate all the data products, thus establishing priorities depends partly on subjective scientific interest. These priorities also reflect knowledge concerning routine availability of correlative data.

Section 5.2.3.3 is a product-by-product discussion of validation plans and issues.

Section 5.2.3.4 summarizes needs for correlative measurements that will not be met by routine observing networks.

Section 5.2.3.5 provides focused plans for a small number of major campaigns in support of Aura validation and science goals. Such campaigns have both defined science goals in their own right and a major thrust towards validation of Aura measurements. Compromise will be required to accommodate needs for correlative data as put forth in sections 5.2.3.3 and 5.2.3.4.

5.2.3.1 Some Specific Issues

5.2.3.1.1 Long-term Validation Issues

Long-term validation plans are important, since satellite data are a primary source for determining global changes and trends in chemical constituents particularly ozone and temperature. Comparisons of trends from Aura data sets for limited geographic regions with trends from data sets obtained using ground-based networks such as NDSC provide validation for the global trends derived from the satellite data. A second component of long-term validation involves comparisons with measurements from other satellite systems that overlap Aura operation for several years.

Time series of HALOE observations of upper stratospheric HCl provide a measure of the effect of international agreements to stop production of chlorofluorcarbons on stratospheric chlorine. The HALOE HCl observations may overlap those to be made by ACE aboard SciSat-1 (mid 2002) and those to be made by Aura MLS. In the absence of significant overlap between these satellites, correlative data is needed for HCl. A series of profiles from balloon-borne instruments would satisfy this need.

Trends in H_2O are also of much interest, but significant differences remain among existing data sets. There is a need for reliable "ground-truth" from a variety of locations, including the tropics.

Some resetting of OMI's calibration parameters is expected after some time, and validation of the revised data will be needed. Some revisions of all Aura instrument calibration and data processing software are also to be expected.

5.2.3.1.2 Coincidence Criteria for Correlative Data

Typical coincidence criteria for stratospheric measurements have been 2 degrees in latitude and 10 to 15 degrees in longitude. This corresponds to roughly 200 km in latitude and 1000-1500 km in longitude at low latitudes, and much smaller longitudinal distances at high latitudes. This loose requirement in longitude reflects the expectation that the atmosphere is more uniform in the longitudinal direction. Acceptable time coincidence for typical stratospheric conditions has been within a day (or "on the same day").

Tropospheric data require better temporal and spatial coincidences between satellite and correlative data. Coordination of radiosonde, ozonesonde, and balloon/aircraft flights will be needed, along with possible coordination with other networks, such as NDSC. Tighter criteria are also necessary to validate horizontal structures that will be revealed by HIRDLS and OMI. OMI plans to use assimilation techniques to increase the statistics for comparisons and meet coincidence criteria.

5.2.3.1.3 Spatial and Temporal Requirements for Correlative Data from Aircraft

The following paragraphs reflect the needs for validation of Aura products from correlative aircraft campaigns. A variety of aircraft platforms should be used to probe the lower troposphere through lower stratosphere.

TES measurements will emphasize the troposphere where the spatial and temporal variability of trace species is much larger than in the stratosphere. This is due to the large variability in the sources and sinks of some species, the short chemical lifetimes of species such as O_3, NO_x and NO_y in the lower troposphere, and the spatial non-uniformity induced by large-scale weather systems. These effects provide a severe test of the TES retrieval algorithms. Ozone is the only species for which there is an observation-based climatology in the troposphere, and even for ozone, our knowledge of its distribution is poor in the northern tropics [Logan, 1999; Oltmans et al., 2001; Thompson et al., 2001]. The data record for NO, NO_2, HNO_3, and CO is limited to the results of previous aircraft campaigns. Mean profiles have been formed for a number of regions from an aggregation of these data [Emmons et al., 2000]. Correlative data that span a wide range of tropospheric conditions will be required for these species. Concentrations of NO_x span 3 orders of magnitude, while those for CO a factor of 10, excluding the most polluted urban conditions. Profiles are often highly layered.

There are a few key parameters that introduce significant variability in the TES Level 1B nadir spectra. These include the profiles of atmospheric temperature and water vapor, the surface cover type, the skin temperature, and cloud and aerosol properties such as temperature, emissivity, coverage and composition. There is also significant variability in the mixing ratios of biogenic and anthropogenic trace species. The result is that the retrieval algorithm will frequently encounter significant differences between the *a priori* and observed spectra, resulting in possible convergence problems. It is therefore necessary to obtain a large number of validation data sets over widely varying conditions to test the flexibility of the retrieval fully.

Table 5.4 summarizes the broad categories of geophysical variables and conditions that should be sampled in the troposphere. These include latitude (tropics, mid-latitudes and high latitudes), pollution level (clean/background, moderate and heavy) as defined mainly by CO and NO_x, surface cover (water, grassland, desert, forest, ice/snow), and cloud/aerosol contamination (clear, cirrus/haze). Wide latitude coverage is important for validation studies because of the associated variability in land cover and temperature and water vapor profiles. Pollution levels should vary from clean to heavy pollution as a test of retrieval stability and convergence under conditions of large optical depth changes. Cloud and aerosol loading should vary to test the ability of the algorithm to reject contaminated scenes and/or retrieve cloud and aerosol properties as the algorithm becomes more mature.

Table 5.4. Ranges of Observing Conditions for TES Nadir Validation Measurements

Latitude	Pollution Level	Surface Cover	Cloud/Aerosol	Number of Observations
Tropics	Clean Moderate Heavy	Ocean Grass Forest Desert	Clear Cirrus Haze	24
Mid-Latitudes	Clean Moderate Heavy	Ocean Forest Grassland	Clear Cirrus Haze	18
High Latitudes	Clean Moderate	Snow/ice Forest	Clear Cirrus Haze	8
			TOTAL	50

In Table 5.4, "observation" is defined as a group of several (three or more) vertical profile measurements of the TES primary species which are spatially and temporally coincident with Aura overpasses. While the coincidence criteria are dependent on factors such as winds, proximity to source regions, etc... a working definition of "coincidence" is 4 hours and 100 km in time and space, respectively. To facilitate the acquisition of overpasses that are coincident with aircraft spirals, TES can be commanded to operate in a special mode in which the nadir footprints are contiguous.

The table shows that a relatively large number of validation measurements are required to sample the range of geophysical variables that will affect the TES retrievals. It is likely that many of of the TES validation objectives can be met with fewer than 50 observations. For example, it may not be necessary to obtain validation measurements in clean oceanic air in both the tropics and mid-latitudes.

As discussed in section 5.2.3, major tropospheric aircraft campaigns such as those fielded by the NASA GTE Program are limited in spatial and temporal coverage and will probably not meet the requirements given in Table 5.4. While the measurement capabilities of fully instrumented aircraft such as the DC-8, P-3 and ER-2 are considerable, and will be very valuable for Aura validation, they will have to be supplemented by smaller, targeted aircraft campaigns that address specific needs such as upper tropospheric odd nitrogen and CO.

For aircraft validation, TES could be operated in the transect mode, in which the footprints are contiguous. Several aircraft transects will be required within each footprint to average the horizontal and vertical inhomogeneity. Each validation sortie would probably require a day's worth of measurements. A minimum number of such correlative data sets (days) is required (see Table 5.4); these should be obtained under cloud-free conditions (except for those specifically meant to address cloud effects).

There are other Aura retrievals of tropospheric and lower stratospheric constituents (see Fig. 3.1) for which validation campaigns from aircraft will be needed. For OMI tropospheric ozone and NO2 column densities, aircraft measurements comparable to those for TES are needed; aircraft campaigns (with, for example, UV/VIS DOAS type instruments aboard) measuring tropospheric and stratospheric partial columns and profiles of ozone and NO_2 will be very useful. For the HIRDLS and MLS retrievals (as well as for limb retrievals from TES), the footprints (averaging regions) are significantly larger than for the TES nadir views. The spacing between profiles is also larger (see typical patterns discussed in section 2.2.5), of order 150 km (MLS) to 500 km (HIRDLS), although HIRDLS may use different modes of observation in order to optimize the overlap with correlative aircraft underflights. Several flights along the Aura measurement tracks, covering a minimum of 1000 km will be needed to provide sufficient statistics for the Aura measurements with strong enough signal-to-noise for good single-profile retrievals (Table 5.3). A range of atmospheric conditions should be tested during such campaigns, with initial emphasis on quiet conditions, to test different conditions for the retrievals and to optimize both science and validation needs. Homogeneity over the averaging footprints of Aura measurements is desirable for simpler comparisons. The number of different conditions desired for HIRDLS and MLS correlative data is not as extensive as indicated for the TES nadir measurements above, but about 4 flights probing the various altitudes of interest is considered a minimum – for a typical campaign, over a time period of a few months.

We would like to have the aircraft flights coincide in time with the Aura measurements. We realize that the time needed for data gathering from aircraft is significantly longer than the time required by Aura instruments to accumulate several atmospheric profiles over a particular region (see also section 5.2.3.1.3). Thus we seek to make correlative measurements when constituents are not varying rapidly either spatially or temporally.

5.2.3.2 Correlative Measurement Priorities

The following subsections are the Aura instrument team guidelines for priorities of correlative measurements, but they need to be folded in with specific science goals to arrive at recommended choices for major campaigns in support of Aura measurement validation and science (see section 5.2.3.5). A more general listing of Aura-wide priorities for correlative measurements is given in the summary section 5.3. This listing provides fewer details in terms of altitude dependence and reflects the overall Aura science goals given in section 2.1.

5.2.3.2.1 Correlative Measurement Priorities for HIRDLS

The correlative measurement priorities for HIRDLS (Table 5.5) have been guided by consideration of the scientific importance of the upper tropospheric and lower stratospheric region (UT/LS), the spatial and temporal variability in the UT/LS and the relative paucity of global observations in this region.

Table 5.5. HIRDLS Validation priorities.

Priority	Geophysical Parameter	Comments
1	Altitudes: $z < 20$ km (1) O_3, H_2O, HNO_3, aerosols (2) CH_4, N_2O (3) Cirrus cloud and PSC properties, heights and locations	Frequent measurements of (1) including vertical profiles and horizontal gradients. Measurements of (2) and (3) less often.
2	Altitudes, $z < 20$ km NO_2, CFC-11, CFC-12, T	
	Altitudes: 20 km $< z <$ 50 km (1) $ClONO_2$, HNO_3, NO_2, N_2O_5 (2) Aerosols, PSC, T, O_3 (3) CH_4, N_2O, CFC-11, CFC-12	Constrained by previous observations and simultaneous observations with TES, MLS, other satellite instruments.
3	Altitudes: $z > 50$ km (1) CO_2 (2) T, O_3, H_2O	Correlative data difficult to obtain in this altitude region.

Validation of structure in HIRDLS measurements

An important focus of the HIRDLS measurements is the ability to resolve globally features in atmospheric temperature and constituents on a scale smaller than has previously been possible from space (about 1.5 km vertically, 250 km horizontally). Validation of these features in the atmosphere is a special challenge because they can be localized and highly variable in time. Exact coincidences in space and time between ground-based and satellite measurements are unlikely. Features like gravity waves can appear quite different in in-situ measurements from an aircraft platform than in satellite limb measurements which represent an average over hundreds of km horizontally along the line-of-sight. For example, gravity waves viewed by HIRDLS along a surface of constant phase might appear as a large perturbation, while if viewed perpendicularly might be invisible. Profile measurements via lidar or balloon soundings also sample a relatively small volume of atmosphere compared to the satellite so that the comparison suffers similar difficulty. The best direct validation of these features must come from high-altitude aircraft observations with flight paths designed to map out the horizontal structure on the scale of the HIRDLS measurement footprint. Observations from balloons will be useful to define the vertical structure.

Comparison of statistical properties of the features in the HIRDLS data with those of other data sets is an indirect method of validation. In the stratosphere, statistical properties of vertical features in HIRDLS data may be compared with the statistical properties derived from observations from the global networks of balloon soundings for validation of both temperature and ozone. The SPARC project of the WMO is compiling such statistics for features in radiosonde temperature measurements globally. Comparison to profiles obtained via refraction of GPS signals should also be very useful for validation of vertical temperature structures. These comparisons also require a statistical treatment unless the lines-of-sight between the two satellite measurements are nearly coincident. In the mesosphere, lidar measurements may be used in this way, and comparison to SABER measurements from the TIMED satellite may be possible. Comparison of features in global models with observed features will be used to validate the HIRDLS data through examination of processes like isentropic mixing and gravity wave propagation.

5.2.3.2.2 Correlative Measurement Priorities for MLS

Table 5.6 illustrates the priorities set by the MLS team for validation needs of the MLS geophysical data products. These priorities were developed considering the scientific importance and uniqueness of the measurements, the difficulty and novelty of the measurements for MLS (measurements from stronger emission lines may require less corroboration with correlative data) and the likely amount of routine correlative data available for a particular product.

Table 5.6. MLS Correlative Measurement Priorities. Measurements are listed in approximate order of decreasing priority within each category.

Priority	Geophysical Parameter	Comments
1	Upper tropospheric O_3, CO, H_2O, T	Aircraft measurements (preferably of vertical profiles) along the MLS track would be especially valuable, particularly in the tropics. Tropical data (e.g. sondes) would also be especially valuable (O_3, H_2O).
	Lower stratospheric O_3, H_2O, OH, BrO, HCl, N_2O, HNO_3 (and SO_2, if large volcano erupts into the stratosphere).	Aircraft measurements along the MLS track, vertical profiles if possible. Balloon/sonde measurements of vertical profiles.
	Upper tropospheric cloud data: number density and particle size distribution (for sizes of ~100 μm up to 1 mm), and total ice density.	Measurements for clouds above ~8 km in the tropics (along the MLS measurement track if possible).
2	Upper tropospheric HCN	
	Lower stratospheric ClO, HOCl, T Lower stratospheric HO_2, CO	Polar winter data needed for chlorine species. Vertical profiles needed.
	Middle/upper strat. OH, HO_2, BrO, HCl, ClO, H_2O, O_3, HNO_3, N_2O, HOCl, CO, T	Vertical profiles needed.
3	Stratospheric HCN, CH_3CN, SO_2 (if no large volcanic eruption), geopotential height	Vertical profiles needed.

5.2.3.2.3 Correlative Measurement Priorities for TES

The goal of the TES validation activity is to validate all standard products listed in Section 3.2.3.2. Temperature, H_2O and O_3 profiles have the highest priority. Tropospheric ozone is a major focus of the TES experiment. Validation of temperature and H_2O is particularly important in the troposphere because retrieval of all other products depends on the accurate determination of these two parameters. Table 5.7 summarizes the correlative measurement priorities for TES.

Table 5.7. TES Correlative Measurement Priorities.

Priority	**Geophysical Parameter**	**Comments**
1	Tropospheric O_3, H_2O, T	O_3 is of major scientific interest. Knowledge of H_2O & T affects all other products.
	Tropospheric CO, NO, NO_2, HNO_3	NO and NO_2 are mainly upper tropospheric products.
	Stratospheric O_3, H_2O, N_2O, CH_4, HNO_3	
2	Tropospheric CH_4	CH_4 is better mixed than other TES products.
	Stratospheric NO, NO_2, CO	
3	TES Special Products	See Table 3.7. Some of these products will be measured routinely by other Aura instruments, and have higher overall Aura priority (e.g., $ClONO_2$).

The primary challenge for validating tropospheric and lower stratospheric parameters is to account for the spatial and temporal variability of the atmosphere. A statistical approach, where many correlative comparisons are appropriately averaged, may be required to achieve an accurate assessment of the TES data products. For all of the TES standard data products there are several in-situ measurement techniques with adequate precision and accuracy for the validation of TES products. Over half of the TES vertical range is accessible with high altitude aircraft.

Figure 5.4 illustrates some of the variability issues. The figure shows ozone in the 0 - 7 km altitude range measured by the NOAA Aeronomy Laboratory by in-situ sampling aboard a NOAA P3 Orion and an ozonesonde profile, all recorded on July 11, 1995, near Nashville, TN. The measurements were made as part of the 1995 Intensive Campaign of the Southern Oxidants Study [Meagher et. al., 1998]. The aircraft measurements were made by flying a series of ~100 km long east-west flight lines, each at a different altitude, about 50 km south of downtown Nashville, TN. The data were acquired over a period of about 1.5 hours starting at about noon. The sonde was released at noon near downtown Nashville. Ozone along the flight lines (lines of constant altitude on the longitude line) varies by as much as ±15 ppbv or by about 25% of the mean. The altitude range of these measurements is somewhat less than two TES vertical resolution elements for nadir retrievals. Variability in the altitude is even greater than in the horizontal and must be properly accounted for in any comparisons between correlative measurements and TES data.

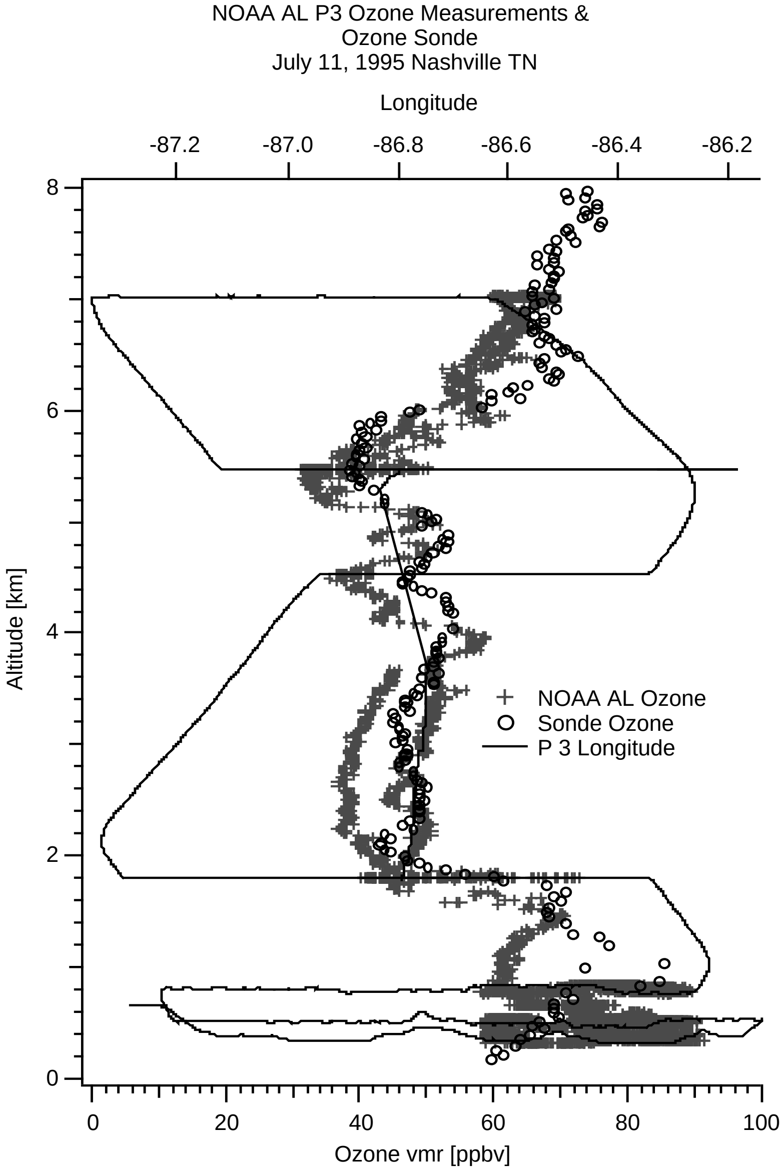


Fig. 5.4. Ozone profiles measured near Nashville, TN, in July, 1995.

TES validation of temperature, water vapor and ozone

Radiosondes will be the primary source of correlative data for validation of TES temperature and water vapor, while ozone sondes will be the primary source of correlative data for ozone. Sondes are emphasized because they cover the entire TES latitude range with high vertical resolution, at least for temperature and ozone. Coincidences between radiosonde and TES profiles are expected to be frequent, allowing statistical description of comparisons, and temperature profiles are readily available for locations over much of the globe. Coincidences between ozonesondes are TES are expected to be infrequent, and we show below that coordinated releases will be required. Comparisons between TES and radiosonde profiles can be made routinely on a daily and continuous basis. Meteorological analysis fields such as those provided by the ECMWF and the DAO are not useful for TES validation because these will likely be used as first guesses for the TES retrievals. The general approach for comparing sonde profiles to TES profiles is to smooth the sonde profiles with the TES retrieval averaging kernels, and then to accumulate averages and standard deviations of the difference between the smoothed sonde and TES profiles. This approach was used for the validation of temperature for UARS ISAMS [Dudhia and Livesey, 1996] and CLAES [Gille et. al., 1996].

TES temperature and H_2O

For temperature and water vapor TES will use data from the global radiosonde network used for numerical weather prediction (see section 5.2.2.1). While there are many details to be worked out, the intent is to gather daily sonde profiles that meet coincidence criteria and compare average differences between sonde and TES profiles over regions. The number of coincidences per day depends on the coincidence criteria, and it is anticipated that there will be between 50 and 100 daily comparisons. Because met sondes are launched at 0000 and 1200 GMT the locations of coincidences will be somewhat geographically isolated. The criteria for coincidence between the sonde and TES profiles need to be studied . They are likely to be different for temperature and water and may vary with location. AIRS (on Terra) requires coincidence within 100 km and 1.5 hr; this allows about 30 coincidences a day. The radiosondes provide reliable water vapor data only to about 150 hPa (or higher pressures), depending on the sensor used (see Section 5.2.2.3)

TES ozone

Ozonesondes are released only once a week at most stations, usually on Wednesdays. We investigated the likelihood of coincidences between sonde releases and Aura overpasses, for the sonde stations that provided data to WOUDC or to the SHADOZ program for 2000. This calculation used the Aura orbit characteristics, and assumed that sondes are launched weekly on Wednesdays. Results are shown in Table 5.8. The first column gives the total number of Aura overpasses within 150 km of an ozonesonde station for each latitude band in 32 days, the second column gives the number of days with an Aura overpass on which a sonde is released from any station in the latitude band, and the third column gives the number of stations per latitude band. The situation if most favorable for high latitudes, with 14 sonde launches coincident with overpasses per month, corresponding to 3-4 coincidences at each station. At mid-latitudes, there would be 24 days in total each month when a sonde was launched on the same day as an overpass. However, at any one station, there are generally only 0-2 coincidences per month, except for the two stations which release sondes 3 times per week for which there would be 5 days per month with coincidences.

In the tropics there are many fewer Aura overpasses within 150 km of the sonde stations, and even fewer on days with a sonde launch. Table 5.8 shows that there would be only 3 coincidences per month with sondes from the 9 SHADOZ stations, with no coincidences at most stations. If the overlap radius is increased to 250 km, there would be a total of 8 coincidences with sondes in a month, but no coincidences at 5 of the 9 stations. It will be essential to have high quality tropical sonde data available for TES validation, and this need could be met by continuation of the SHADOZ program. However, sonde launches would need to be coordinated with Aura overpasses to be able to build up a reasonable data base for validation. Coordinated releases would also be desirable at selected mid-and high-latitude stations, to build up good statistics for validation.

The accuracy of ozonesondes is adequate (5-10%) if proper sonde procedures are used. We will take advantage of new information on sonde accuracy and precision from recent studies in the Jülich Ozone Sonde Intercomparison Experiment (JOSIE) [Smit and Kley, 1996; unpublished results, 2001], and from other recent experimental studies.

Table 5.8. Frequency of overpass coincidences with ozonesonde stations, within 150 km.

Latitude range	Coincidences with Aura per 32 days	Number of days with sonde launches per 32 days	Number of stations
90N-60N	162	14	4
60N-30N	110	24	12
30N-0	15	2	2
0-30S	53	3	9
30S-60S	9	1	1
60S-90S	20	3	1

TES validation of CO, NO, NO_2, HNO_3

More information regarding the validation approach for these and the other TES products is provided in section 5.2.3.3.

5.2.3.2.4 Correlative Measurement Priorities for OMI

OMI's first task is to continue to monitor column ozone over the entire globe. Ozone column densities and ozone profiles are therefore the most important OMI Level 2 products. Since direct monitoring of industrial pollution and biomass burning is another main goal of OMI, the validation of ozone and NO_2 total and tropospheric column densities and profiles, and of aerosols is also high priority. Retrieval of the main Level 2 products depends on cloud information, thus cloud properties must be validated carefully with correlative measurements. For HCHO, there are few opportunities to obtain correlative measurements. Campaign efforts could be used to improve this , using in situ instruments on airplanes or groundbased UV/VIS spectrometers (see Table 5.1)

Because of OMI's wide swath, daily global coverage is achieved for all data products. Collocation with ground-based observations at any location can be achieved by coordinating measurement times with the OMI overpass time.

All OMI retrieval algorithms rely on the measurement of the Earth's reflectance. Since most of the radiation registered by the OMI detector is backscattered at relatively high altitudes, 'looking' deep into the troposphere is difficult. Validation of tropospheric concentrations is therefore very important. Another important aspect of retrieval techniques employed by OMI is the sensitivity to the Airmass Factor (AMF). Determination of the AMF is difficult when solar zenith angles are large, thus validation at high latitudes is very important. The AMF also depends on *a priori* information. Large variations in the AMF occur during high aerosol loading in the troposphere (in smog-areas at midlatitudes, and biomass burning regions in the tropics), with high cloud cover, or when there is a lot of ozone variation in the troposphere (which occurs in the tropics as well). Thus validation of OMI data will depend upon correlative data obtained at high latitudes and in the tropics.

Correlative measurement needs are as follows:

- **Ozone:** airborne measurements of tropospheric profiles (nadir-viewing) and stratospheric profiles (zenith-viewing) are needed in biomass or industrial areas, for validation of the tropospheric ozone column densities, and their horizontal variability.
- **NO_2:** measurements are needed in the tropics, industrial and biomass burning areas, where high NO_2 amounts are expected (tropics and industrial regions). NDSC-instruments do not meet this need, as they are often located at elevation or/and in relatively clean areas. NO_2 column densities and amounts of NO_2 in the first few km of the troposphere are strongly linked, thus to validate

measurements in polluted areas, ground-based and airborne measurements of NO_2 profiles are needed. Campaigns, including aircraft measurements, should provide these. Although OMI derives column densities, profile shapes are needed for a validation of the assumptions about the altitude distribution of NO_2 that are made, which influence the NO_2 column density strongly. Possibilities for instruments are groundbased lidar (location Bilthoven, the Netherlands, pending funding) or UV/VIS photometers relocated to strategic locations.

- **Aerosols:** the measurements by OMI can be validated using the existing Aeronet network. However, campaigns should provide in situ measurements of aerosol size distribution, chemical composition, index of refraction, absorption and extinction to test algorithm assumptions.

Table 5.9 summarizes the correlative measurement priorities for OMI.

Table 5.9. OMI Correlative Measurement Priorities.

Priority	Geophysical Parameter	Comments
1	O_3	Airborne measurements of tropospheric (nadir-viewing) and stratospheric (zenith-viewing) profiles are needed, especially in the tropics.
	NO_2	There is a clear need for measurements of NO_2 profiles, and total and tropospheric column densities in areas with enhanced NO_2 levels (e.g., industrial regions, tropics). Strong need for airborne measurements.
	Clouds	Cloud heights should be validated, note that pixel size and collocation are important issues.
	Aerosols	In situ measurements of aerosol size distribution, chemical composition, absorption and extinction would be very valuable, especially in regions like South-East Asia.
	SO_2 under volcanic conditions	
2	BrO, OClO, HCHO, UV fluxes, UV-B	
3	SO_2 background	

5.2.3.2.5 Summary of Correlative Measurement Priorities for Aura

Priorities for validation of the planned Aura measurements are summarized below. Validation need, the perceived importance of a quantity to addressing science goals, and further discussion among Aura investigators were considered in assigning priority. The numbering scheme chosen here (1 for higher priority, 2 for medium priority, 3 for lower priority) is also used later in this document (see Tables in summary section 5.3). This may be used as a rough guide to design of correlative campaigns. We recognize that Aura team members would like to be able to fully validate all Aura measurements, but we also recognize that some atmospheric measurements are more difficult to validate and that the scientific importance is not equal among measurements.

Stratospheric Measurements

Priority 1: Temperature, O_3, H_2O, N_2O, CH_4, HCl, OH, HNO_3, BrO, SO_2 (if large volcanic eruption)

Priority 2: ClO, $ClONO_2$, CFC-11, CFC-12, HOCl, HO_2, NO, NO_2, N_2O_5, CO

Priority 3: HCN, CH_3CN, SO_2 (if no large volcanic eruption), geopotential height

Ozone is a high priority constituent, but the large amount of correlative data in the stratosphere from satellite instruments and ozonesondes weakens the need for additional correlative profile data. Issues related to horizontal variability are discussed below as part of campaign needs. Temperature errors can have a significant impact on retrievals of other Aura products, but, as for ozone, correlative observations are routinely available. Other high priority constituents include H_2O (for lower stratospheric processes and stratospheric trends), N_2O and CH_4 (tracers and greenhouse gases), HCl (for the upper stratospheric total chlorine trend; also a new MLS measurement), OH (a key stratospheric radical and new MLS measurement), HNO_3 (for denitrification and nitrogen budget issues), BrO (part of the ozone depletion/recovery issues and a new MLS measurement).

Tropospheric Measurements

Priority 1: Temperature, O_3, H_2O, CO, HNO_3, NO, NO_2

Priority 2: CH_4, and upper tropospheric N_2O, CFC-11, CFC-12 , HCN

Priority 3: geopotential height (upper troposphere)

Most of the tropospheric measurements from TES are given high priority because they will provide unique global data sets. Priority 2 constituents including CH_4 are not expected to exhibit as much variability as other constituents such as CO.

Column Density Measurements

Priority 1: NO_2, NO_2 (tropospheric), O_3, O_3 (tropospheric), SO_2 (if large volcanic eruption)

Priority 2: HCHO, OClO, BrO

Priority 3: SO_2 (if no large volcanic eruption)

O_3 and NO_2 columns by OMI are given high priority because they will provide a unique daily global tropospheric data set. For ozone, it is important to validate the horizontal variability in the troposphere, using airborne measurements. For NO_2, tropospheric column and profile information under polluted conditions is necessary since the NO_2 columns are largely determined by the contribution of the troposphere.

Measurements of Aerosols, PSCs, Clouds, UV fluxes

Priority 1: Aerosols, PSCs, Clouds

Priority 2: UV fluxes (for OMI)

Aerosols, clouds, and PSCs are part of the ozone depletion/recovery issues. Furthermore, aerosol and PSC spectral information is needed to improve retrievals for other Aura products. Aerosol validation will be of more importance in the event of a large volcanic eruption.

5.2.3.3 Validation Approach for each Aura Data Product

A brief discussion is presented below for the comparison and validation activities for each of the main Aura products. These are listed according to priority as given above. Aerosols and clouds are discussed for the stratosphere and troposphere following the discussion of priority 1 column density measurements. More detailed planning and implementation will occur before the Aura launch. When possible, we provide guidelines for reference data sets. Intercomparisons among Aura instruments do not by themselves constitute validation; correlative data sets with demonstrated high quality are required. Post-launch activities that would validate many of the constituents measured by Aura are summarized in Section 5.3

PRIORITY 1 STRAT. TEMPERATURE AND TRACE GAS MEASUREMENTS

Temperature [stratosphere, TES, HIRDLS, MLS]

Although there is an abundance of routine correlative data for temperature (especially at northern mid-latitudes), inclusion of temperature data in validation campaigns (aircraft and/or balloon-based) is important since temperature errors affect the quality of constituent retrievals for Aura products.

Reference data sets

1 Operational Meteorological data sets such as the products from DAO, NCEP and UKMO represent the most likely validation sources.
2 GPS temperature profiles may be available in 2003-2004 in sufficient numbers and with accuracy comparable to or better than radiosondes, with possibly better coverage in the Southern Hemisphere.
3 Other candidates including AIRS are listed in Table 5.3.

Long-term validation: Sufficient non-Aura high quality data should exist (as mentioned above) to carry out this phase of the validation studies for temperature.

O_3 [stratosphere, HIRDLS, MLS, OMI, TES]

Ozone profiles are measured by various satellite instruments, and by ground-based instruments throughout the world. Well-validated measurements with good absolute accuracy (within 5-10%) throughout the stratosphere are provided by NDSC primary stations (sondes, stratospheric lidars, microwave sensors). For the altitude region below 30 km, sonde measurements are available for 20^o-80^o N (e.g. from WOUDC), with more limited data available for other latitudes. Continuation of the SHADOZ program would ensure availability of profiles for the tropics. To achieve global coverage, measurements by Aura will be compared with measurements from various satellite sensors (Table 5.3).

Aircraft-based ozone lidar profiles (above and below the aircraft) should enable validation of horizontal gradients along the orbital tracks (MLS and HIRDLS).

Reference data sets:

1 SAGE profiles (Table 5.2); for near global coverage and for initial quality checks, SCIAMACHY data or assimilated SCIAMACHY ozone fields. Other satellite data sets are listed in Table 5.3; expected periods of operation for the satellites are given in Table 5.2.
2 Although not global in coverage, NDSC primary sites and some complementary sites since this network provide the most accurate and reliable measurements of ozone profiles.

Long-term validation: SAGE and ENVISAT data, combined with ground-based profile data for the stratosphere (e.g., from ozonesondes, lidars, microwave instruments), will provide comparisons towards long-term validation of stratospheric O_3. Other ozone-measuring satellite experiments planned during the Aura timeframe are listed in Table 5.2.

H_2O [stratosphere, HIRDLS, MLS, TES]

Reference data sets: There is no easy choice, given the range of measurements for stratospheric H_2O, but profiles from balloon-borne instruments are the most likely candidates. Such profiles are needed outside of northern mid-latitudes. Ground-based microwave profiles (e.g., NDSC sites) will be utilized as well, but not for the lower portions of the stratosphere.

There will be several satellite data sets with which to compare, including HALOE (if available in 2003-2004), SAGE III, ODIN, SABER, ENVISAT instruments, and ILAS-II (Table 5.2). Other data sets, including AIRS and AMSU, are listed in Table 5.3.

Long-term validation: A series of stratospheric balloon flights is needed. Combination of several satellite datasets with those from the Aura instruments should provide a significant database for stratospheric H_2O and its long-term variations.

N_2O [stratosphere, HIRDLS, MLS, TES]

Reference data sets: Satellite instruments measuring profiles of N_2O include MIPAS, ILAS-II, ACE, and ODIN (Table 5.2). SCIAMACHY will provide N_2O profile information from about 20 to 40 km. Ground-based FTIR and microwave instruments provide column and profile data (respectively) in limited locations. Climatological data derived from UARS observations provides a baseline for assessing seasonal and latitudinal behavior.

Long-term validation: N_2O measurements from aircraft (in situ whole air sampling and spectroscopy, FTIR) and balloons (in situ gas chromatography) augment the data sources outlined above.

CH_4 [stratosphere, HIRDLS, TES]

Reference data sets: Balloon profiles provide the best reference data sets. Data from satellite instruments HALOE (if still available), SCIAMACHY, MIPAS, ILAS-II, and ACE will be investigated.

Long-term validation: Comparisons with measurements throughout the course of the Aura mission are desirable, especially since there have been significant variations/trends in methane in the stratosphere.

HCl [stratosphere, MLS]

Reference data sets: Profiles from UARS HALOE (if operational) would be an excellent reference data set. ACE (aboard SciSat-1) would be another choice (launch planned in 2002), if the data have already undergone a significant amount of validation. Balloon IR data (campaigns and/or 2 or more flights per year) would provide profiles for validation.

Long-term validation: Intercomparisons among data from satellite instruments (MLS, HALOE, ACE) and spot checks from non-satellite data will be utilized; a series of stratospheric balloon flights is needed.

OH [stratosphere, MLS]

Lower stratospheric aircraft data during stable atmospheric background conditions such as observed at mid-latitude equinox during polar summer (because of H_2O and O_3 influence on OH) could be compared with zonal mean data from MLS.

The MLS signal strength is useful for single profile retrievals in the upper stratosphere, and balloon data for OH profiles would be very valuable for comparisons throughout the stratosphere.

The solar zenith angle dependence compared to model expectations for latitudes/seasons when MLS measurements get close to polar night conditions is a useful comparison. This test can only be made at high latitudes since the MLS observations at other latitudes are made at fixed local solar conditions, day or night.

Comparisons versus ground-based OH column data would help build statistics, and would be useful for longer-term validation studies as well (even without resolution of the vertical profile).

Long-term validation: Ground-based column OH data are the best source for (at least first-order) validation of the MLS OH profiles (and column values). A series of stratospheric balloon flights is needed.

HNO_3 [stratosphere, HIRDLS, MLS, TES]

Reference data sets: Profiles from balloon flights and ground-based instruments (microwave and infrared) are needed for validation. A sufficient database for validation can be obtained during the first 2 years after Aura launch. Vertical profiles may be obtained by remote sensing balloon-borne spectrometers operating in the middle-IR by solar occultation and emission, far-IR emission and microwave/submillimeter emission. In the lower stratosphere, HNO_3 measurements have been made on aircraft using chemical ionization mass spectroscopy.

UARS MLS and ODIN will provide climatological data and profiles for comparison if the instruments are operational after Aura launch (Table 5.2). Other satellite instruments expected to observe HNO_3 during the Aura time frame are MIPAS, ILAS-II and ACE.

Long-term validation: Issues of possible increases in denitrification in the polar regions play a role in the science goals for stratospheric HNO_3. In addition to the satellite data mentioned above (intercomparisons), we would like to compare the Aura data to timeseries of HNO_3 profiles from NDSC sites. A series of polar stratospheric balloon flights is needed.

BrO [stratosphere, MLS]

Reference data sets: Balloon in situ instruments and SCIAMACHY are the main sources of data for comparisons (Table 5.3). MLS data will be averaged to produce monthly zonal means. We plan to maximize the use of balloon flights for stratospheric profile validation; latitudinal gradients that appear in the satellite BrO data could be used to plan correlative balloon flights at different latitudes.

Long-term validation: Comparisons with SCIAMACHY are the best possibility for long-term validation efforts. Spot checks from balloon flights for consistency are necessary.

SO_2 (volcanic) [stratosphere, MLS]

Reference data sets: If there is a significant volcanic SO_2 input into the stratosphere, balloon data and SCIAMACHY data would provide a basis for validation. Column data from OMI and TOMS will be compared with the integrated profiles.

PRIORITY 1 TROP. TEMPERATURE AND TRACE GAS MEASUREMENTS

Temperature [troposphere]

Reference data sets: See above discussion of stratospheric temperature. In addition to operational meteorological data sets such as the products from DAO, NCEP and UKMO, individual radiosondes and/or ARM data offer the best coincidence and are a good choice for the troposphere.

O_3 [troposphere, TES, HIRDLS, MLS, OMI]

Reference data sets: Ozonesonde profiles will provide the main source of validation. The need for data in the tropics can partly be met by continuation of the measurements in the SHADOZ program (5.2.2.1). However, for assessment of the horizontal variability of O_3, and validation of the OMI tropospheric column densities in general, airborne campaigns are needed (e.g., with a UV/VIS DOAS type instrument on board) in biomass burning or industrial areas. In the upper troposphere, satellite sensors that may provide O_3 profile measurements globally during the Aura timeframe include SAGE, ODIN, SABER, ENVISAT and ILAS-II. We will utilize several of these data sets for validation.

Long-term validation: For the troposphere, comparisons with data at fixed sites (mainly ozonesonde sites) will be used to build statistics. Averaged MOZAIC aircraft data will be utilized as well.

H_2O [troposphere, TES, HIRDLS, MLS]

Reference data sets: The network of humidity sondes provides a good global data set with frequent measurements (typically once to twice per day), from the ground up to about 150 hPa. For pressures less than 300 hPa, we would preferably use Vaisala RS-80H or RS-90 humicap sensors as reference, because of their demonstrated accuracy. We plan to investigate better coincidences because of the variability in the troposphere, although even with very good time coincidences, the measurement footprint of some of the Aura instruments will be a limitation. The ARM data sets will be used as well.

Profiles of H_2O and other Aura products from troposphere to lower stratosphere should be measured from aircraft flying along the Aura tangent track as part of campaigns.

Other data sets including AIRS and HSB are listed in Table 5.3.

Long-term validation: Analyses based on radiosonde data provide long-term validation for tropospheric humidity data.

CO [troposphere, MLS, TES]

Reference data sets: Carbon monoxide profiles have been measured during campaigns as part of the NASA Global Tropospheric Experiment (GTE). Averaged profiles derived from these data are given by Emmons et al. [2000], while the archived data are available from the Langley DAAC or from http://www-gte.larc.nasa.gov. The GTE data are for altitudes 0-12 km. Data for higher altitudes from NASA ER-2 missions are described by Herman et al. [1999].

The MOPITT validation program is providing bimonthly aircraft profiles of CO from five sites. Canisters are collected on light aircraft that reach 7-8 km.

The MOZAIC program is starting to make regular CO measurements in 2001, and should provide a useful database from the ground to 12 km.

Necessary Correlative Measurements. Measurements must be planned to validate CO retrievals over a wide range of concentrations (40 to several hundred ppb), with vertical structure anywhere from relatively uniform to highly layered. This variability is a consequence of the short lifetime of CO (weeks in the tropics and mid-latitude summer) coupled with the spatial and sometimes temporal heterogeneity of CO sources. Vertical profiles from the ground to the tropopause will be essential for TES validation. This can be accomplished by conventional aircraft in midlatitudes, but will require high-flying aircraft or balloon measurements in the tropics. The complement of instruments used for MOPITT validation will be applicable to TES data. This includes the regular aircraft profiles described above. Ground based solar FTS measurements of the CO column are also being used for MOPITT validation. Measurements from the surface flask network are not particularly useful for TES validation.

It is unlikely that two major tropospheric campaigns will provide sufficient profiles for TES validation, as discussed in Section 5.2.3, although the high resolution CO profiles provided by these campaigns are an essential part of the validation strategy. An additional set of coincident profiles will be required, with an aircraft that can reach 12 km. Flask sampling from such an aircraft would give sufficient temporal and vertical resolution for satellite validation, and the samples also provide measurements of other needed species such as CH_4 and N_2O. It is important that all in-situ measurements can be related to the same calibration standards. MOZAIC aircraft flights should provide correlative data up to about 12 km, but these commercial flights cannot be timed for coincidences with satellite overpasses.

HNO_3, NO, NO_2 [troposphere, HIRDLS, MLS, TES, OMI]

Reference data sets. The climatologies of NO_x and HNO_3 in the global troposphere are poorly characterized. HNO_3 and NO profiles have been measured on the NASA/GTE campaigns, with the addition of NO_2 since 1996. Average profiles derived from these data are given by Emmons et al. [1997, 2000] and Thakur et al. [1999] while the archived data are available from the Langley DAAC or from http://www-gte.larc.nasa.gov.

Necessary Correlative Measurements. As with CO, tropospheric NO, NO_2 and HNO_3 concentrations vary over a wide range, from a few ppt to several ppb with vertical profiles that range from uniform to highly structured. The sources of tropospheric NO_x are spatially non-uniform and include combustion, biomass burning, lightning and stratospheric intrusion. While NO_x lifetimes are generally quite short (hours to days) the lifetimes of HNO_3 are longer (days to weeks). NO and NO_2 therefore exhibit significant diurnal variability, in contrast with HNO_3.

TES measurements of tropospheric NO, NO_2 and HNO_3 can be obtained in the limb mode only. The TES detection limits for these species are somewhat uncertain. For example, the detection of tropospheric NO is complicated by factors such as departures from LTE in the stratosphere and mesosphere. However, measurements of NO and NO_2 at the 100 ppt level should be possible to the middle troposphere. The measurement of HNO_3 in the 10-50 ppt range should be possible throughout most of the troposphere.

Vertical profiles from the middle troposphere to the tropopause will be essential for TES validation of NO and NO_2, and from the surface to the tropopause for HNO_3. For validation of OMI NO_2 tropospheric column densities, profiles starting at ground level will be needed (this is described in detail in the NO_2 column density validation section). This can be accomplished by conventional aircraft in midlatitudes, but will require high-flying aircraft or balloon measurements in the tropics. Instrumentation capable of ppt or sub-ppt measurements of NO_x are not required for TES validation. Small instruments which place fewer requirements on the platform (mass, power) are appropriate for TES validation, and will permit more frequent measurement opportunities. Large tropospheric measurement campaigns such as INTEX and LARS/TRACE-B (section 7.C) will provide high resolution data sets for NO_x and a number of species in the NO_y family. For proper validation of TES data however, these missions must be supplemented by smaller missions which take place several times per year. These "mini-missions" do not need to provide measurements at the state-of-the-art detection levels for NO_x but must be properly calibrated and intercompared.

NO [troposphere, TES]

Troposphere: See write-up (above) for tropospheric HNO_3.

NO_2 [troposphere, HIRDLS, TES, OMI]

Troposphere: See write-up (above) for tropospheric HNO_3. For OMI, see write-up for NO_2 column densities.

PRIORITY 1 COLUMN DENSITY MEASUREMENTS

NO_2 Column Densities [OMI]

Several satellite platforms provide global measurements of NO_2 column densities. Their sensitivity for the lowest part of the atmosphere, however, is limited. Ground-based UV/VIS spectrometers (DOAS and SAOZ, data contained in NDSC database) and FTIR measurements also provide column densities, at various sites with reasonable global coverage. However, they do not cover polluted areas well (see below).

An important issue is the contribution of tropospheric NO_2 to the column densities. As was described in the tropospheric HNO_3, NO, NO_2 section, NO_2 profile climatologies poorly characterize the actual NO_2 profile shape, especially in areas with severe pollution. Many ground-based instruments within NDSC are located at elevation, or in relatively clean areas, where little tropospheric NO_2 is expected. Since OMI wants to measure tropospheric and total column densities of NO_2 under various circumstances, including biomass burning and industrial pollution, additional measurements of tropospheric NO_2 under polluted conditions are needed. This calls for campaigns in industrial or biomass burning regions (using airborne or balloon measurements), employing, e.g., UV/VIS DOAS type instruments. An additional possibility is to use correlative lidar measurements, from a ground-based NO_2 lidar located at RIVM (Rijksinstituut voor Volksgezondheid en Milieu – i.e. Dutch Institute for Public Health and the Environment) Bilthoven, the Netherlands (52°N). At this location, moderate to high NO_2 concentrations in the lower troposphere are expected (note: operation is awaiting funding sources).

Another important issue for the NO_2 validation is its diurnal variability. NO_2 is destroyed rapidly in the presence of sunlight, and thus concentrations during OMI overpasses will differ from those measured by ground-based techniques which measure most accurately at sunrise and sunset. Measurements coincident with OMI overpasses are preferred, if these can have sufficient accuracy. Existing techniques can be applied for small solar zenith angles but give less accurate results than at sunrise/sunset.

Since tropospheric NO_2 is highly variable in the horizontal direction, networks in which the NO_2 concentrations at the ground are measured are useful when used in conjunction with models predicting the height of the boundary layer. Under the assumption that NO_2 is distributed homogeneously through the boundary layer, and that the free troposphere contains little NO_2, the tropospheric NO_2 loading can be determined with about 50-100% uncertainty. Knowledge of the horizontal distribution of NO_2 in the boundary layer is important for the validation itself but also for checks of the assumptions made (i.e., the airmass factor depends strongly on the amount of boundary layer NO_2).

Reference data sets:

(1) SCIAMACHY, GOME

(2) ground-based UV/VIS and FTIR, preferably NDSC extended with instruments in polluted areas. NDSC stations in Japan are at low elevation and in polluted areas. Feasibility of using daytime FTIR spectra for NO_2 column retrievals should be investigated.

(3) additional campaign-based UV/VIS and FTIR (DC8 airborne measurements of NO_2, or balloon-based UV/VIS spectrometers)

(4) possibly ground-based lidar (The Netherlands)

(5) ground level measurements (SOS etc...) combined with boundary layer height predictions from meteorological data

Long-term validation:

Same data sets as above, with addition of NIWA long-term measurements (45°S, 170°E, clean troposphere) [Liley et al., 2000].

O_3 Column Densities [OMI (and HIRDLS, MLS, TES)]

Measurements of the ozone column densities take place worldwide within the Brewer-Dobson network. Reported instrument accuracy of 5% can be improved slightly if the temperature dependence of these results is taken into account (see, e.g., Brinksma et al. [2000]). Measurements are taken almost daily. Also, various satellite instruments measure ozone column density data. For the Aura instruments, it is necessary to distinguish separate stratospheric and tropospheric columns. It is expected that additional correlative tropospheric O_3 column data are needed during biomass burning events, when O_3 concentrations are high and variable.

Reference data sets:

1 during campaigns: airborne lidars used for profile comparisons should be incorporated in the OMI O_3 column density validations
2 ozonesondes for tropospheric partial column validations
3 existing Brewer-Dobson network for column density validations
4 existing satellite instruments for column density validations

Stratospheric column densities: MLS and HIRDLS should initially plan to compare stratospheric column values versus SAGE data, as well as ozonesonde data.

Total column densities: The OMI total column ozone will be validated versus existing ground-based column data (e.g., the Brewer-Dobson network); analyses will make use of data assimilation for increasing the statistics of comparisons. TOMS, GOME and SCIAMACHY data will be utilized for validation purposes.

Tropospheric column densities: This product can be estimated from OMI data, along similar lines as was done for TOMS and GOME data, or from a combination of OMI, and HIRDLS or MLS data. Ozonesondes are the best current data source at several sites, including the tropical regions. Comparisons are planned with other tropospheric products derived from TOMS and SCIAMACHY data; these products do not have the precision of sonde-derived columns, especially outside the tropics, but they provide a more global picture.

Campaigns are envisaged for regions where tropical ozone has high variability, e.g., polluted or biomass-burning areas. Airborne lidar measurements (with lidars pointing upward as well as downward) will yield profiles throughout the troposphere and stratosphere, typically at about 100 locations per flight.

Long-term validation: There is a significant amount of high quality data from ground-based networks for O_3 column densities for long-term validation; TOMS and SCIAMACHY data can also be used (Table 5.2). For the stratospheric column densities, validated profiles would be used (see above notes). Tropospheric products will rely heavily on ozonesondes for long-term validation.

SO_2 column (volcanic) [OMI, TES (and MLS)]

Because SO_2 is short lived in the troposphere, background concentrations are small and in the absence of a volcanic eruption SO_2 columns can only be detected in the immediate vicinity of a source. Validation of SO_2 under non-volcanic conditions is described in the priority 3 section (below). Sources are volcanic passive degassing and combustion of sulfur-rich fossil fuels. Validation of background SO_2 retrievals will require surface or airborne column measurements in the vicinity of these sources.

The validation of SO_2 column densities in volcanic eruption clouds is problematic because the timing of eruptions is unpredictable and the trajectories of the clouds cannot be forecast accurately. In the past, chance passages of SO_2 clouds over Brewer instruments have provided validation for satellite observations.

Brewer spectrophotometers, COSPEC (correlation spectrometers), and UV/VIS measurements from the ground are the primary validation sources for the SO_2 vertical column densities. Use of these is not entirely satisfactory as the accuracies of these methods have yet to be reviewed accurately. In addition, the methods have not been intercompared, although and COSPEC instrument intra-comparisons have been made. Other satellite instruments, such as TOMS, MODIS, ASTER, SCIAMACHY and GOME 2 provide global correlative observations. Integrated MLS vertical SO_2 profiles can be compared with column measurements for large volcanic clouds.

Reference data sets:

1 UV/VIS SO_2 column densities from ground-based DOAS instruments.
2 Brewer network SO_2 column amounts in archived data sets
3 COSPEC special campaigns on active volcanoes (e.g., Popocatepetl)
4 TOMS SO_2 and ash data record on eruptions
5 Validated SO_2 column densities from ASTER, MODIS, SCIAMACHY and GOME 2 (if available)

Long term validation: SO_2 emissions are episodic with extremely high variability due to volcanic eruptions.

PRIORITY 1 MEASUREMENTS OF AEROSOLS, PSCs, CLOUDS

Aerosols, PSCs, Clouds [HIRDLS, TES]

HIRDLS and TES emission measurements will include contributions by stratospheric sulfate, polar stratospheric cloud (PSC), and tropospheric cirrus particles. Since atmospheric emission is due to opacity from both gaseous and particulate species, the error budget of the gaseous retrievals is partly determined by how well the retrievals can account for aerosol effects. Trend studies of gaseous species will be impacted especially if a major volcanic eruption occurs during the Aura mission. Following a general discussion of issues related to validation of the Aura measurements of particle properties, validation issues for these different types of particles are discussed sequentially.

General comments:

Cloud and aerosol particle effects depend on composition (i.e. wavelength dependent indices of refraction), particle size distributions (the number of particles per unit volume per radii interval), and particle shape (e.g. H_2SO_4/H_2O droplets are spherical, PSC and cirrus particles can be non-spherical). The effects of particles also depend on the geographical distribution of the particles, since PSC and upper tropospheric cloud particles can occur in localized layers. It is possible to have several types of particles present along the line-of-sight. Multiple scattering effects may present further complications.

Heterogeneous chemistry calculations require particle area and volume densities, quantities not measured directly by emission experiments but dependent upon retrievals.

The validation of aerosol effects and aerosol characteristics is accomplished using several different types of measurements. TES and HIRDLS will inter-compare radiation fields for latitudes and seasons where the type of particle is expected to differ, for example sulfate at middle latitudes and PSCs at winter high latitude. The HIRDLS instrument functions can be applied to TES emission spectra to derive altitude dependent radiance profiles for the HIRDLS channels. Radiance profile comparisons for the different regions for these two instruments will be carried out periodically.

The second level of validation deals with aerosol extinction profiles. HIRDLS extinction profiles and TES extinction profiles, which are a research product, will be inter-compared at common wavelengths for different conditions (mid-latitude stratosphere, polar regions, upper troposphere).

The third level of validation is inter-comparison of derived products such as volume and area density. These non-standard special products are dependent upon retrievals. The theoretical and observational limitations of these retrievals need to be assessed using optimal estimation techniques, and the values need to be compared to in-situ measurements. Area and volume densities are readily calculated from particle size distributions that are measured by balloon-borne and aircraft instrumentation.

The simplest retrieval of area and volume density utilizes fits to scatter plots of extinction versus volume density, and extinction versus area density, where the density values are calculated using an ensemble of size distributions measured previously by in-situ instruments. The calculations can be based upon Mie calculations for spherical particles, and indices of refraction of known materials (e.g. H_2SO_4/H_2O, ice, NAD, NAT etc...). It is desirable to develop retrievals of area and volume densities, and perhaps idealized size distributions, using multiple wavelength extinction data and optimal estimation techniques.

Other Satellite platforms:

The POAM III, HALOE, and SAGE III experiments (Table 5.3) will retrieve aerosol extinction data that will be very useful for Aura aerosol validation. HALOE aerosol extinction wavelengths are 2.45, 2.8, 3.4, and 5.26 μm, and the POAM and SAGE wavelengths range from 0.353 μm to 1.55 μm; also, POLDER on ADEOS-II or on Parasol and GLAS on ICESat should provide aerosol and cloud information at 0.4 to 1.1 μm. HIRDLS and TES observe in the infrared and the other instruments mentioned above observe at shorter wavelengths. Extinction data for the various experiments will be intercompared with wavelength dependent Mie calculations that utilize correlative measurements of altitude dependent particle size distributions and laboratory measurements of wavelength dependent indices of refraction.

ILAS II will measure aerosol extinction at high latitude via solar occultation at 0.78, 7.16, 8.27, 10.6, and 11.76 μm. Extinction measurements at 7.16 and 8.27 μm are very similar to the HIRDLS aerosol channels 13 (8.20-8.33 μm) and 19 (7.06-7.13 μm).

The GOMOS and SCIAMACHY instruments to be flown onboard ENVISAT measure aerosol extinction profiles from about 0.25-0.950 μm and 0.28-2.3 μm, respectively. Their vertical resolution is lower than that of the solar occultation instruments mentioned above, but they will have global and night-time coverage. Comparison to HIRDLS and TES extinction measurements will require Mie calculations to account for the differences in observational wavelengths.

Sulfate aerosol (background):

If there is no major volcanic eruption during the Aura time frame, then infrequent measurements of the sulfate layer in the stratosphere at mid-latitudes are acceptable. Seasonal measurements of the size distributions of sulfate particles from balloon borne instrumentation are required. These measurements are used in Mie calculations to estimate the magnitude and spectral wavelength dependence of the sulfate aerosol.

Lidar measurements (e.g., from the NDSC network) of spatial inhomogeneity of the sulfate layer are also required, since spatial variations partly determine how well in-situ measurements can be compared to limb observations that integrate over a several hundred km path length. The shape of lidar backscatter profiles and extinction profiles measured by HIRDLS and TES (research product) can be compared after wavelength-dependent Mie calculations convert the backscatter to extinction, or vice-versa. The fine vertical resolution of the lidar measurements is useful to evaluate the HIRDLS and TES altitude registration (e.g. when comparing sharply peaked volcanic or PSC layers).

Sulfate Aerosol (major volcanic event):

If a major eruption occurs, then monthly balloon-borne particle size distribution measurements are desirable during the first year or two after the eruption to track changes in the particle size distribution, and also provide values for the volume and area density. Coordination of the balloon flights with Aura overpasses is necessary. Lidar measurements of the representative spatial variations of the aerosol cloud will be very useful. Retrievals will need to account for these multiple scattering effects present after a major volcanic event. MLS observations will not be affected by a major volcanic cloud.

Polar stratospheric clouds:

PSCs occur in the polar regions at low temperatures, and the extinction is higher than that of the background sulfate aerosol. Some PSCs are made of liquid solutions of nitric acid, sulfuric acid and water. Others are made of solid nitric acid hydrates (e.g. NAD and NAT), and others are water ice. Each of these is expected to have a different infrared signature, not only because their optical properties differ but also because they have different characteristic particle sizes. The TES experiment is especially well suited to retrieve PSC aerosol spectra, since aerosol optical depths can be retrieved in numerous wavelength micro-windows.

PSCs are particularly difficult to validate. Several particle types can coexist in localized regions, the geographical distribution of PSCs varies on spatial scales smaller than the several hundred km integration length of the satellite limb view, and radiative transfer in the vicinity of PSCs is complicated (e.g. non-spherical particles, multi-scattering effects, etc...).

Both cold sulfate and PSC particles contribute to chlorine catalyzed loss of ozone by serving as sites for heterogenous reactions that convert reservoir constituents HCl and $ClONO_2$ into more reactive forms. Background or volcanically enhanced sulfate particles can be distinguished from PSC particles based upon the wavelength dependence and magnitude of the aerosol extinction. This will be an important part of understanding the ozone changes over the next decade if lower the lower stratospheric temperatures decrease, changing either the frequency or duration of PSCs or the importance of sulfate to chlorine partitioning. Retrieval efforts to determine the spectral signature and area density of PSCs, in conjunction with correlative measurements of the area density values and composition, are important tasks, since it is the combination of surface area, composition, and cold temperature that drives heterogeneous chemistry.

Measurements of particle size distribution and composition are needed to understand details concerning PSC particles development and evolution, and to quantify representative number, area, and volume densities. Measurements by lidar instruments of the spatial variations and the polarization characteristics of PSCs are desired, since the polarization measurements identify particle shape differences (e.g. ternary droplets are spherical while hydrate crystals are non-spherical).

Tropospheric cloud particles:

Cirrus and cloud particles will produce extinction that is measurable by TES and HIRDLS, though thick clouds will limit where and when retrievals are possible in the troposphere. These observational limitations are important, since cloud systems transport chemical species from the lower to the upper troposphere. If the retrievals are located only in clear sky regions, Aura data will not fully characterize upper tropospheric mixing ratio gradients, in relation to locations of deep convection.

The HALOE (UARS) and MODIS (Terra) currently measure upper tropospheric cirrus distributions. The MIPAS interferometer, the ESSP3 (PICASSO-CENA) active satellite lidar experiment, the SAGE III occultation experiment, and the ACE interferometer will measure upper tropospheric cirrus distributions during the Aura mission (POLDER on Parasol and ICESat/GLAS may also contribute). MODIS radiometer channel data identifies the horizontal location of opaque clouds.

Background tropospheric aerosol:

In-situ sampling of aerosol in the upper troposphere has indicated that the aerosol can contain organic material. The composition of the upper tropospheric aerosol therefore is likely more varied than that of the stratospheric sulfate layer. In-situ composition and size distribution measurements of the upper tropospheric background aerosol are needed to better understand the optical properties of the aerosol extinction that will be sensed by TES, OMI, and HIRDLS in cloud free conditions.

Long-term Validation: Continued comparisons with the data sets noted above will be useful/needed. Measurements of the particle size distributions of volcanic aerosol particles will be necessary if a major volcanic eruption occurs during the Aura lifetime, since the aerosol extinction will then vary by a factor of 100 in the infrared.

Aerosols [OMI]

OMI will derive aerosol optical thickness and single scattering albedo. In situ measurements of aerosol properties are also needed to validate the assumptions that have to be made in deriving aerosol quantities. Most of these measurements are only made during campaigns, however, some stations perform them more regularly. These measurements include:

1 aerosol size distribution measurements
2 measurements of the chemical composition of the particles
3 aerosol absorption measurements
4 aerosol scattering measurements

Aerosol Optical Thickness (AOT)

OMI will retrieve the AOT for cloud free pixels only. We will rely primarily on AERONET for the AOT data taken by ground-based sun photometers. Other important validation sources include ground-based lidar systems and space-based lidars like ESSP3 (PICASSO-CENA) and GLAS. AOT measurements by satellite instruments will be used for intercomparison purposes only.

Reference data sets:

1 AERONET ground-based sunphotometer measurements.
2 Ground-based lidar measurements
3 Space-based lidar measurements from ESSP3 (PICASSO-CENA) and possibly GLAS
4 Validated AOT measurements taken by satellite instruments (if available): SCIAMACHY, MODIS, TOMS, POLDER, MISR.

Long-term validation:

Comparisons with the AERONET data will be most useful for long-term validation purposes.

Aerosol Single Scattering Albedo (ASSA)

OMI will retrieve ASSA for cloud-free pixels only. We will primarily rely on AERONET for the ASSA data taken by ground-based sun photometers, although it is not certain that the measurements by AERONET will give single scattering albedos that are accurate enough to be useful for validation of the OMI single scattering albedo. For the derivation of single scattering albedos from OMI, good cloud masks and good ground albedo information is needed, and therefore validation of these products is desired.

Reference data sets:

AERONET ground-based sun photometer measurements.

Long-term validation:

Comparisons with the AERONET data will be most useful for long-term validation purposes.

Cloud Ice Content [MLS]

Estimates of ice and liquid particle size distributions for sizes of ~100μm up to 1mm are needed for various conditions in the upper troposphere, especially for clouds above ~8km in the tropics. Gathering climatological data sets is to be completed pre-launch. Aircraft and/or balloon correlative measurements of the above cloud properties will support MLS validation and data interpretation efforts and could also support validation of CloudSat data. Ground-based radar and lidar will also supply correlative data.

MLS plans to validate its estimates of cloud ice water content (and extinction) mainly through comparisons with data from the CloudSat CPR (Cloud Profiling Radar). The CPR will provide high resolution cloud ice content values (500m vertical resolution on 4km x 1.5km footprints that will need to be integrated over the coarser MLS sampling volumes. This comparison will be possible if Aura and CloudSat satellites fly in formation as discussed in section 5.2.2.3.

The AIRS HSB nadir data (with a footprint size of order 10-20km) provide radiance measurements at 183 ±1, ±3, and ±7 GHz, which can be used to compare with the MLS 177-183GHz limb radiances. Such comparisons will be useful for validating the radiative transfer model and retrieved cloud parameters.

MODIS and MERIS: High-resolution cloud coverage and cloud top height estimates from these (and other infrared/visible satellite) instruments will be particularly useful for validating the MLS cloud ice product. Since the MLS algorithm needs to estimate an effective cloud top height before the cloud ice retrieval, such input and validation from other instruments will help MLS to constrain possible error sources.

In addition, validation data would be desirable from aircraft and/or balloon upper tropospheric measurements (especially for clouds above 8 km in tropics) of

Long-term validation: CloudSat data should provide the best data for validation of cloud ice content. Validation of CloudSat data itself will also take time during the Aura timeframe, but this is not a big drawback, as the ice content product from MLS will not be part of the initial production processing.

Cloud coverage and cloud top height [HIRDLS, TES]

Cloud measurements are not the primary focus of Aura, but information about clouds will help refine (or flag, initially) the Aura retrievals of chemical composition. The occurrence of clouds in the fields of view of the 4 Aura instruments will affect these retrievals both above and below the clouds (to varying degrees, depending on the instruments and the cloud types).

OMI will measure cloud coverage and cloud scattering pressure with a fine horizontal resolution. These measurements should be of value to the other Aura instruments; their validation plans are described in the sections below.

The CloudSat 95 GHz cloud profiling radar will obtain 0.5 km vertical resolution measurements of the distributions of clouds. ESSP3 (formerly PICASSO-CENA) flying in tandem with CloudSat (with launch planned for after mid-2003) has a 2-wavelength (532 and 1064 nm) lidar that will obtain accurate cloud top heights.

Several other EOS-era instruments will obtain measurements of cloud properties. The AIRS/AMSU instrument will measure the fractional cloud coverage, cloud top height, type, and cloud top temperature. CERES will measure cloud coverage and cloud top height. The MISR multi-angle data set will provide studies of cloud type and height (from Terra). MODIS (on Terra and Aqua) will also provide cloud coverage and cloud top pressure.

Ground-based techniques such as meteorological radars should provide some useful correlative data regarding clouds, if the space and time coincidences with Aura overpasses occur in very narrow windows (given the variability of cloud fields); sufficient statistics will be needed for the determination of biases between these ground-based and satellite-based datasets. We note that CloudSat and ESSP3 (PICASSO-CENA) will fly in close formation with Aura, so that well thought out “ground-based” validation programs should benefit all of these satellite data sets at the same time (section 5.2.2.3).

The use of geostationary satellites, like METEOSAT and GOES, should be evaluated.

Cloud Properties [OMI]

Effective Cloud Fraction (ECF)

Most of the Level 2 OMI data products depend on the quality of the (internal) effective cloud fraction product. Validation of the effective cloud fraction should therefore be interlinked with that of other products.

A first test could be to substitute the OMI effective cloud fraction for another cloud product (e.g., the MODIS cloud fraction) and study the sensitivity of the retrieved OMI products for this. However, this does not take away the need for intercomparison of the cloud products to those measured by other instruments.

Among primary sources for intercomparison, we will consider the ESSP3 (PICASSO-CENA), CloudSat and MODIS cloud fractions. Their horizontal resolution needs to be taken into account. The WMO Network may provide valuable information since it produces cloud fractions that have been measured with a different, independent technique. Other validation sources include the SCIAMACHY and ATSR-2 visible radiances cloud cover product.

Reference data sets:

1. Validated ESSP3 (PICASSO-CENA), CloudSat and MODIS cloud fractions
2. WMO Network
3. Validated effective cloud fractions from SCIAMACHY and ATSR-2 visible radiances cloud cover product (if available)

Long-term validation:

Comparisons with ESSP3 (PICASSO-CENA), CloudSat, MODIS, and GOME II would be most useful for long-term validation.

Cloud Pressure [OMI]

Most of the Level 2 OMI data products depend on the quality of the cloud pressure. Validation of this data product is difficult, since the dependence of cloud pressure on the instrument spectral region changes when cloud density and cloud thickness change. On the other hand, comparisons between different instruments can indicate under which circumstances the cloud pressure derived from OMI can be interpreted to have a physical meaning.

The strategy to validate cloud pressure must rely on comparisons with cloud top pressures derived from similar spectral regions as used for OMI. The most important satellite instrument employing a different technique (lidar altimetry) while staying near the OMI spectral region (at 532 nm) is PICASSO-CENA. Other satellite instruments that may be useful for intercomparison include AVHRR and SCIAMACHY, and in a later stage possibly GOME II.

Internal validation will take place between the cloud pressures derived from OMI measurements by the two different methods used: O_2-O_2 and Raman bands.

Reference data sets:

1. Cloud top pressure from MODIS, AVHRR, and SCIAMACHY.
2. Validated cloud top pressure from PICASSO-CENA (if available)

Long-term validation:

Comparisons with ESSP3 (PICASSO-CENA) as well as with CloudSat would be useful for long-term validation.

PRIORITY 2 STRATOSPHERIC MEASUREMENTS

ClO [MLS]

Reference datasets: UARS MLS (if operational) will provide a reference data set. Good precision in the enhanced conditions of the winter/spring polar vortex makes single profile comparisons possible. Climatological data from UARS MLS can be used for first-order comparisons. ODIN satellite microwave data will also be used for comparisons (Table 5.2).

Ground-based sites offer microwave profiles from several locations (e.g., NDSC sites). Like UARS MLS, Aura MLS ClO profiles will require averaging during non-enhanced conditions, which favors comparisons with ground-based profiles observed during stable atmospheric conditions.

Balloon and aircraft profile measurements would also be valuable data sets. Both microwave data and in situ data are desirable. The latter offer high vertical resolution and precision through a very different measurement technique.

Long-term validation: Validation studies will focus on comparison of time series of ground-based microwave profile retrievals with time series from Aura MLS. Aircraft and/or balloon-borne data would be utilized as well, if a fairly consistent longer-term record is available. Consistency is expected as first-order validation with observed trends both in HCl (MLS, ground-based instrumentation, HALOE and/or ACE (if either is operational)), and CFCs (HIRDLS, ground-based data).

$ClONO_2$ [HIRDLS]

Reference data sets:

1 $ClONO_2$ will be measured by satellite instruments including MIPAS, ILAS-II, and ACE (Table 5.2). If suitably validated these observations will be useful references for HIRDLS. ILAS-II comparisons will be valuable in the winter and spring at high latitudes, where $ClONO_2$ concentrations vary dramatically due to polar stratospheric cloud chemistry.

2 Total column data from several NDSC sites (ground-based FTIR) can be used to check for overall consistency.

3 Photochemical model calculations will be used to compare observed diurnal behavior of $ClONO_2$, with expectations.

Long-term validation: Balloon (FTIR) and aircraft (FTIR, in situ) measurements of $ClONO_2$ will be useful to validate HIRDLS observations, particularly in the lower stratosphere. A series of stratospheric balloon flights is needed.

CFC-11 [HIRDLS]

Reference data sets:

1 Validated data from satellite instruments such as MIPAS aboard Envisat, ILAS-II, and ACE aboard Sci-Sat should be available for comparison (Table 5.2).

2 Climatological data from UARS CLAES might also be useful, although the projected decrease in CFC-11 abundance would need to be accounted for.

Long-term validation: In situ (e.g., gas chromatograph or grab samples) and remote (e.g., airborne FTIR) observations from balloons and aircraft would be most useful for long-term validation.

CFC-12 [HIRDLS]

Reference data set:

1 Validated data from satellite instruments such as MIPAS aboard Envisat, ILAS-II, and ACE aboard Sci-Sat should be available for comparison (Table 5.2).

2 Total column data from NDSC sites (ground-based FTIR) can be used to check for overall consistency.

3 Climatological data from UARS CLAES might be useful, although the projected decrease in CFC-12 abundance would need to be accounted for.

Long-term validation: In situ (e.g., gas chromatograph or grab samples) and remote (e.g., airborne FTIR) observations from balloons and aircraft would be most useful for long-term validation.

HOCl [MLS]

MLS data will be averaged to produce monthly zonal means. Balloon IR data are a possible source of HOCl profiles for comparison. Comparison of observations with model expectations is a likely path for first-order validation.

Long-term validation: We expect to use a first-order validation approach based on expectations for HOCl abundance using observed and/or modeled ClO and HO_x variations.

HO_2 [MLS]

MLS data will be averaged to produce monthly zonal means. The comments for OH (above) serve as a guide for HO_2 validation, although there are fewer possible sources of correlative data for HO_2.

NO [TES]

Reference data sets: The only remote sensing technique for validation purposes is mid-IR solar occultation spectroscopy (e.g. Mark IV spectrometer). Since there is significant diurnal variability in NO profiles, comparison of these measurements with the TES emission measurements will involve a diurnal correction. In situ measurements of stratospheric NO have been made at altitudes up to 40 km using the O_3 chemiluminescence method [e.g., Kondo et al.] and long-path diode laser absorption [e.g., Webster et al.]; these techniques remove (to a large extent) the issue of diurnal variation for the comparisons.

Satellite data of interest would be HALOE (if still operational) and ACE (if available and validated), although diurnal corrections would be needed because these instruments measure during sunrise or sunset.

NO_2 [HIRDLS, TES]

Reference data sets: Vertical profiles of interest may be obtained by remote sensing balloon-borne spectrometers operating in the UV/visible region (limb solar scattering or nighttime lunar/stellar absorption), middle-IR (solar occultation, e.g. Mark IV) and middle-IR (emission e.g. MIPAS). In situ measurements of stratospheric NO_2 have been made using balloon-borne long-path diode laser absorption spectroscopy and by laser-induced fluorescence in the lower stratosphere. NO_2 has a significant diurnal variation in the stratosphere that will place constraints on the temporal and spatial sampling in validation studies and/or entail the use of model-derived diurnal corrections, at least for occultation data.

Also, a large number of satellite data sets (see Table 5.3) should be available for comparison with the Aura NO_2 observations.

N_2O_5 [HIRDLS]

Reference data sets: N_2O_5 will be measured by other satellite instruments including MIPAS and ACE. If these observations are suitably validated, they will be useful as references for HIRDLS.

Other analyses:

As diurnal behavior is important in N_2O_5, comparisons to photochemical model calculations, constrained by simultaneous observations of NO_2, will be important.

Long-term validation: There are limited options for measurement of N_2O_5, except by remote sensors such as ATMOS and balloon- or aircraft-borne FTIRs. Observations from these instruments in a variety of photochemical environments (high and low latitudes, cross-terminator) will be extremely useful in validation of the HIRDLS N_2O_5 product.

CO [MLS, TES]

Reference data sets: Balloon profiles provide the best reference data sets. The number of profiles is limited by balloon launch possibilities. CO does not have a large diurnal variation, so either the far-IR balloon emission spectrometer of Carli *et al.* or the mid-IR solar occultation spectrometer (Mark IV) of Toon *et al.* could provide satisfactory validation profiles. SCIAMACHY and ODIN (Table 5.2) may provide global data sets for CO.

Long-term validation: Consistent long-term measurements from non-satellite platforms are needed. Intercomparisons among satellite data sets (SCIAMACHY, MLS, TES) will probably provide the best test of relative changes.

PRIORITY 2 TROPOSPHERIC MEASUREMENTS

CFC-11 [HIRDLS]

Reference data sets:

Measurements from the AGAGE network provide ground-level CFC-11 amounts. This is a priority 2 measurement in the troposphere as little variability is expected.

Long-term validation: Comparisons with measurements throughout the Aura mission are desirable, since CFC-11 is expected to show a significant trend.

CFC-12[HIRDLS]

Reference data sets:

Measurements from the AGAGE network provide ground-level CFC-12 amounts. This is a priority 2 measurement in the troposphere as little variability is expected.

Long-term validation: Comparisons with measurements throughout the Aura mission are desirable, since CFC-12 is expected to show a significant trend.

HCN [MLS]

Few observations are available; (upper) tropospheric profiles are desirable, probably via balloon flights (as for the stratospheric values).

CH_4 [HIRDLS, TES]

Troposphere: Many of the comments that are mentioned in the CO section concerning follow-on programs from MOPITT validation missions apply to CH_4. However, the CH_4 concentration is not expected to vary nearly as much as CO, so the need for CH_4 validation is less critical than for CO.

N_2O [HIRDLS, MLS, TES]

Reference data sets:

Measurements from the AGAGE network provide ground-level N_2O amounts for TES. This is a priority 2 measurement in the troposphere as little variability is expected.

PRIORITY 2 COLUMN DENSITY MEASUREMENTS

HCHO Column Densities [OMI]

HCHO slant and vertical column densities are currently measured by GOME [Thomas et al., 1998; Chance et al., 2000; Palmer et al., 2001] and will be measured by SCIAMACHY. Ground- and aircraft-based measurement campaigns will be necessary for OMI validation, especially when concentration are expected to be high, i.e., for periods with strong tropospheric hydrocarbon emissions. A past example is the U.S. Southern Oxidants Study (SOS), measuring continental production of HCHO from isoprene [Lee et al., 1998]. Measurements are also necessary to confirm rates of production in the maritime free troposphere, such as those from the 1997 Subsonic Assessment (SASS) Ozone and Nitrogen Oxide Experiment (SONEX) [Singh et al., 2000]. Measurements over the southeastern U.S. in summertime, and over the midlatitude oceans (preferably in summertime for maximum production from oxidation of CH_4) would provide optimum data sets. Midlatitude maritime measurements could be combined with campaigns to study intercontinental pollution transport.

Reference data sets:

1. Validated HCHO column densities from SCIAMACHY (if available)
2. Validated HCHO column densities from GOME 2 (after 2005)
3. During campaigns, groundbased and aircraft-based data.

Long term validation:

Comparisons with column values from SCIAMACHY would be most useful for long term validation.

OClO Column Densities [OMI]

Limited correlative data is available for the validation of OClO vertical column densities, comparisons to other data should be regarded as intercomparisons rather than validation, since one has to allow for differences in reference spectra and fitting procedures. We regard UV/VIS spectroscopic OClO column measurements from the ground as the primary validation source, since this technique, although similar, is not the exact same as UV/VIS spectroscopic measurements from a satellite platform. Vertically integrated OClO profiles from SAOZ balloons carrying UV/VIS spectrometers will also be used. However, SCIAMACHY and GOME 2 OClO slant and vertical column measurements are valuable validation sources as well since they provide global coverage.

Ground-based correlative measurements must be made over high-latitude locations, where both vortex and outside-vortex conditions are expected.

Reference data sets:

1. UV/VIS OClO column densities from ground-based spectroscopic instruments.
2. Integrated OClO profiles from the Laboratoire de Physique Moléculaire et Applications (LPMA) DOAS data or from SAOZ payloads.
3. Validated OClO column densities from SCIAMACHY (if available)
4. Validated OClO column densities from GOME II (if available)

Long term validation:

Comparisons with the UV/VIS from ground-based measurements and from SCIAMACHY would be most useful for long term validation.

BrO Column Density [OMI, and MLS integrated stratospheric abundance]

Limited correlative data exist for the validation of BrO vertical column densities; comparisons to other data should be regarded as intercomparisons rather than validation, since one has to allow for differences in reference spectra and fitting procedures. We regard UV/VIS spectroscopic BrO column measurements from the ground as the primary validation source; the technique is similar, although not identical, to UV/VIS spectroscopic measurements from a satellite platform. Vertically integrated BrO profiles from SAOZ balloons carrying UV/VIS spectrometers will also be used. SCIAMACHY and GOME 2 BrO slant and vertical column measurements are valuable validation sources as well since they provide global coverage.

Groundbased correlative measurements must be made over high-latitude locations, where both vortex and outside-vortex conditions are expected.

Reference data sets:

1. UV/VIS BrO column densities from ground-based spectroscopic instruments.
2. Integrated BrO profiles from LPMA DOAS data or from SAOZ payloads.
3. Validated BrO column densities from SCIAMACHY (if available).
4. Validated BrO column densities from GOME 2 (if available).

Long term validation:

Comparisons with the UV/VIS from ground-based measurements and from SCIAMACHY would be most useful for long term validation.

PRIORITY 2 MEASUREMENTS OF UV FLUXES

UV-B flux and UV spectra [OMI]

1. "PIXEL" VALIDATION SITES

The scale of UV irradiance variation is related to variability in cloudiness, albedo, ozone and aerosols. The scale of cloudiness variability is on the order of a kilometer. Due to this, it is difficult to compare the spaceborne and ground-based UV data directly. The typical pixel sizes of global spaceborne UV datasets vary between 15 and 320 km. To be able to use ground-based UV data for satellite validation, various measurement sites are needed within a satellite pixel. In this way the validation may be carried out in a physically reasonable way. It is proposed that three validation areas be established for the OMI UV validation. Typically 6 additional simple radiometers/validation areas would be needed. Existing facilities and meteorological know-how will form the basis for the validation areas. The following areas are proposed:

A. SW Finland, 60 N

Existing spectral and broadband UV measuring programme since 1990
Advanced calibration facilities
Snowcover 2-5 months a year
Low aerosol content
High solar zenith angle conditions

B. Greece 30-40 N

Existing spectral and broadband UV measuring programme since 1990
Advanced calibration facilities
High aerosol content, occasionally influence of Saharan dust
High tropospheric ozone content

C. USA sites

Primary: Greenbelt, Md.

- existing spectral and broadband UV measuring programme
(BUV, Double Brewer since 2000)
- calibration site for aerosol AERONET network (SIMEL sun/sky measurements)
- Lidar for aerosol and cloud heights

- spectral UV zenith sky measurements by SSBUV instrument (SKYRAD program)
- UV and VIS shadow-band radiometers from USDA network within 10km.

Secondary: ARM site in Oklahoma

- existing broadband VIS radiation and clouds measuring programme
- UV and VIS shadow-band radiometers from USDA network

2. AIRCRAFT CAMPAIGNS

To study the 3-dimensional distribution of UV irradiance field aircraft measurements are the optimal choice. For OMI validation it would be desirable to install up and down looking UV instruments and possibly also an actinic flux instrument onboard the aircraft that will be used for OMI trace gas validation. The aircraft measurements should be complemented by ground-based instruments in the flight area. The impacts of aerosols, cloudiness, albedo and ozone should be studied. This may be best achieved by carrying out 2-3 campaigns at different environments. Areas of interest are low latitudes with high aerosol loading (dust, biomass burning) and high latitudes with high albedo and strong ozone depletion. Variable cloudiness conditions would be desired for some flights. Potential coordination with the pixel validation activities would be an advantage. The results of the campaigns are expected to be of high scientific value.

3. GROUND-BASED VALIDATION NETWORK

Besides the pixel and aircraft validation activities also long-term UV stations with high-level instrument QA/QC practices are planned to be used in OMI UV validation. Such stations are located in e.g. Europe, USA, Canada, Antarctica and New Zeeland. The data available from European UV Database (FMI), World Ozone and UV Datacentre (AES), NSF Network (Biospherical Inc.) and from individual scientists are planned to be used for long-term OMI UV validation besides the pixel validation areas.

Additional funding is needed for these validation activities. Partial funding may be applied from the European Commission research programmes.

The USDA UV-B Monitoring and Research Program located at Colorado State University has 28 permanent sites located throughout the USA (including Alaska and Hawaii) and 2 in Canada collocated with Canadian Brewers. High quality, annually calibrated and spectrally characterized 7 channel UV shadow-band radiometers measure total, diffuse and direct irradiances every 3 minutes. Nominal wavelengths are 300, 305, 311, 317, 332, and 368 nm (2 nm FWHM). The data is posted on the Web the next day (http://uvb.nrel.colostate.edu/UVB). Aerosol optical depths at 332 nm and 368 nm will also be available on request. To complement the shadowbands, the Network is operating at MD, OK, and CO double UV monochromators with excellent stray light rejection and wavelength repeatability. USDA proposes to share any Network data with OMI as part of the North American ground-based validation network. In addition the Network operates the sites within 150 km and could add several more broadband UV-B and UV-B sensors at additional sites within the spatial array and share the data with OMI.

PRIORITY 3 MEASUREMENTS

HCN [stratosphere, MLS]

Reference data sets:

1. Two or more balloon profiles are sought per year using in situ and remote techniques.
2. NDSC data sets from ground-based instruments (microwave) will be used for comparison. However, these are not as precise in the lower part of the stratosphere as (1), and are therefore less useful.

Long-term validation: A series of stratospheric balloon flights is needed.

CH_3CN [stratosphere, MLS]

Stratospheric CH_3CN, whose primary source is thought to be biomass burning, has been retrieved from UARS MLS data [Livesey et al., 2001], and is planned to be routinely retrieved from the EOS MLS radiances. Monthly zonal means are expected to be the most useful CH_3CN data product, although intense localized enhancements can be seen in individual retrievals. The UARS MLS results indicate a previously undetected peak of CH_3CN in the tropical middle stratosphere (where no measurements have previously been made), suggesting an unknown stratospheric source. Confirmation of this result by in situ techniques (e.g., ion-molecule reaction mass spectroscopy, previously used on aircraft and balloons)

as part of the Aura validation program would be scientifically important and would also benefit the MLS validation for this product (above 100 hPa).
Long-term validation: Comparisons with balloon or aircraft measurements made throughout the course of the Aura mission are desirable.

Geopotential Height (and/or gradients) [stratosphere and upper troposphere, HIRDLS, MLS]
Reference data sets: Operational Meteorological data sets from DAO, NCEP, UKMO and GPS will be considered for comparisons. A tie-in for absolute height (at a given pressure) is required.
Long-term validation: The above data sets should be available and sufficient for the long-term validation purposes.

SO_2 column densities (background) [OMI]
SO_2 background amounts are expected to be less than 0.5 matm-cm over much of the world (Chin et al., 2000). In polluted regions of the northern hemisphere the model results are less than 2 matm-cm. Local amounts near sources are higher but must be averaged over the OMI footprint. OMI SO_2 detection limits will depend on details of the wavelength dependence of the S/N ratio but may be better than 2 matm-cm. The present uncertainty in standard Brewer spectrophotometer SO_2 background amounts is 1 - 2 matm-cm for direct sun data with a well calibrated instrument. Validation of background SO_2 measurements will require special efforts with double monochromator instruments, such as SSBUV or double Brewers.

OTHER CORRELATIVE DATA OF INTEREST TO AURA

Additional correlative data are desirable. These include surface albedo data (at TES and OMI wavelengths) for different regions of the earth.

In addition, as discussed in more detail in section 5.1, OMI expects to use direct solar irradiance measurements from SOLSTICE II, SAGE, GOME 2, and SCIAMACHY several times per year throughout the solar cycle to validate the OMI Level 1 irradiances; GOME 2 and SCIAMACHY radiances will also help in the validation of Level 1 OMI earth radiances. TES intends to use upwelling radiances from a limited number of aircraft and/or balloon data sets as a check of the TES radiances. MLS radiances can be compared to UARS MLS radiances and/or ODIN microwave radiances (if available in 2003), although the MLS team will rely heavily on radiance residuals between observations and calculated forward model to look for potential problems in the radiances or in the retrievals.

5.2.3.4 Summary of Needs for Correlative Data (not met by routine observations)

- Profiles of priority 1 constituents (HNO_3, NO, NO_2, CO, and O_3) are needed throughout the troposphere including the altitude range not normally accessible by conventional aircraft. This calls for dedicated aircraft flights, also because aircraft measurements provide assessments of the horizontal gradients in the constituents measured.
- Tropical ozone profiles and column densities are needed. Maintenance of the SHADOZ network (section 5.2.2.1) partially satisfies this need, but sonde launches must be coordinated with Aura overpasses at some sites (section 5.2.3.2.3). Coordinated launches are also needed at selected mid and high latitude stations.
- Tropospheric NO_2 and O_3 column densities and profiles are needed in polluted regions (priority 1).
- A regular series of balloon launches into the upper stratosphere at middle and high latitudes with appropriate payload is needed, in order to contribute significantly to the Aura validation requirements for priority 1 stratospheric constituents (N_2O, CH_4, HCl, OH, HNO_3, BrO, aerosol extinction), priority 2 constituents (ClO, $ClONO_2$, CFC-11, CFC-12, HOCl, NO, NO_2, N_2O_5), and priority 3 stratospheric constituents (HCN, CH_3CN).
- Ground-based correlative data are needed to validate cloud information from Aura and also CloudSat, ESSP3 (PICASSO-CENA) and MODIS. Necessary cloud information includes the cloud top height, coverage, and particle size distribution. The cloud cover should be known at the OMI pixel size resolution (~10 x 24 km).
- Lower stratospheric OH measured in a stable background atmosphere is needed for comparisons with representative averages from MLS data (priority 1).
- Column densities of BrO, HCHO, and OClO are needed (priority 2).
- Profiles of priority 2 constituents (HCN and CH_4) are needed in the upper troposphere.
- For validation of UV-B flux and UV spectra (for OMI), UV spectrometers should be added to existing aircraft campaigns (priority 2).
- Successful validation of Aura products requires sufficient correlative observations that comparisons of the data sets make statistical sense (section 5.2.5). The troposphere may exhibit large temporal and spatial variability. For some constituents (e.g., lower stratospheric OH), the zonal mean of the Aura measurements must be calculated to reduce noise and improve sensitivity. Creation of an appropriate data base would require regular observations from balloon and aircraft.

5.2.3.5 Campaigns: Where, When, Why?

Campaigns involving coordinated deployment of a suite of instruments from aircraft, balloon, and ground based platforms can contribute significantly to answering scientific questions concerning key issues in atmospheric chemistry and dynamics while fulfilling specific validation requirements of the Aura platform. Ideally, the satellite and campaign data will be used together as equal partners to address science questions.

The following requirements for validation must be kept in mind when developing campaign plans:

- Among the tropospheric Aura products (NO, NO_2, HNO_3 for TES; CO for MLS; H_2O, O_3 for MLS and HIRDLS, trop O_3 and NO_2 columns for OMI), several species are measured only in the upper troposphere, thus high-altitude aircraft and the DC-8 are necessary .
- Correlative profiles with high vertical resolution are of most use when close to Aura profiles in space and time (e.g. along tangent tracks); validation becomes more statistically robust as the number of such cases increases.
- Validation needs require measurements both for quiescent times/places and across sharp gradients (e.g. across the sub-tropics or the winter vortex edge).
- Close coincidences (in space and time) are required, especially for the troposphere.

- The validation needs for certain Aura instruments, TES in particular, will not be met through a combination of the existing ground-based and sonde networks, alone or in combination with large tropospheric aircraft campaigns such as the planned LARS/TRACE-B and INTEX missions. Frequent "mini-missions" that emphasize tropospheric profiling of certain key species (H_2O, O_3, CO, NO, NO_2, HNO_3) over a wide range of geophysical conditions are needed to complement the other validation tools that are available.

A NASA Earth Science Enterprise (ESE) workshop addressing this issue was held August 23-27 1999 in Snowmass, Colorado. Three major themes that could be used to develop campaigns arose: a) water vapor in the upper troposphere and lower stratosphere; b) ozone loss and recovery; c) tropospheric chemistry: greenhouse gases, photochemical oxidants, and aerosols. Clearly these themes relate strongly to the science objectives of the Aura platform discussed in section 2.

There are various arguments to justify validation campaigns in various seasons and locations. Examples are the following:

- Regions with poor coverage (e.g., southern midlatitudes, tropics, Arctic)
- Regions with calm conditions
- Regions with extreme conditions such as temperature
- Regions where retrieval algorithms yield results with limited precision (e.g., tropics due to high clouds and tropospheric ozone variability, or polar regions, due to high solar zenith angle).

The above goals are obviously not compatible with each other, and may not be compatible with science goals attached to a particular campaign. These goals must be prioritized and balance reached. The schematic below is an attempt to address the questions "where, when, why?" in terms of the desirability of validation campaigns. The chart emphasizes the campaign data that would be used in validation of the Aura products.

Campaigns towards Aura Validation

Where?	When?	Why?
(A) Tropics	Aug. – Oct.	trop. O_3, CO (biomass burning) NO_2, aerosols H_2O, T, O_3, cloud properties (stratospheric dehydration, convection dynamics, climate and transport issues)
(B) Polar vortex South is more stable North is more accessible	late winter/early spring	stratospheric O_3 loss + ClO, HCl, HNO_3, H_2O, ...
(C) Midlatitudes balloon-borne profile data	near equinox	mainly for Aura stratospheric products e.g., OH, HO_2, NO, NO_2, HNO_3, N_2O_5 ClO, HCl, $ClONO_2$, HOCl, BrO, Aerosols + longer-lived species
(D) Continental outflow regions or industrial/ biomass burning regions	during outflow maximum (generally summer)	tropospheric chemistry O_3, CO, NO_x, HNO_3, ...
(E) Areas with high lightning incidence (e.g., S. Florida)	summer	lightning as source of NO_x, HNO_3

There are other possibilities for campaigns with obvious links to the overall science questions for the Aura platform presented in section 2.1.1. Campaign suggestions, measurements that would be useful to address the topics, and also latitudes, seasons, and altitude ranges in which the measurements should take place are given below for each of the four main questions directly relevant to Aura measurements.

- **Is the ozone layer changing as expected?**

Topic: Different types of PSCs and their role in denitrification in the northern hemisphere winter vortex.
Rationale: Climate change may lead to a colder northern vortex and higher stratospheric water mixing ratio. Either or both of these may affect polar stratospheric cloud formation and denitrification processes, ultimately leading to more intense ozone loss in the northern hemisphere than has been experienced to date.
Measurements proposed: balloon *in situ* measurements of O_3, NO_2, OClO, BrO,
aerosols, PSCs, including particle size and composition,
tracer profiles inside and outside the vortex. Also, ground-based aerosol and ozone/temperature lidar, routine ozonesondes
northern winter high latitudes

Topic: Lifecycle of the Antarctic ozone hole, and trends in early winter ozone depletion at the vortex edge
Rationale: The chemical destruction of ozone within the Antarctic vortex may become greater if the size of the vortex changes due to climate change
Measurements proposed: aircraft and balloon *in situ* measurements of NO_2, OClO, BrO,
aerosols, PSCs including particle size and composition
ground-based aerosol and ozone/temperature lidar
routine ozone sondes
southern winter high latitudes

Topic: Relationship between ozone column density at SH midlatitudes, tropopause altitude, and stratosphere/troposphere exchange
Rationale: To clarify the role of changes in the tropopause altitude on long term ozone trends
Measurements proposed: ground-based aerosol and ozone/temperature lidar
routine ozone sondes
southern midlatitudes, all seasons

- **Do we understand the transport of gases within the stratosphere and between the stratosphere and troposphere?**

Topic: Tropical exchange between the troposphere and the stratosphere
Rationale: To clarify mechanisms that control the mixing ratio of stratospheric H_2O and the mechanisms that determine the altitude of the tropical tropopause
Measurements proposed: Tropical profiles of O_3, H_2O and temperature, cloud top height
All seasons

Topic: Horizontal and vertical transport processes near transport barriers (subtropics and winter vortices)
Rationale: To clarify mechanisms that cause and maintain separation of stratospheric air masses
Measurements proposed: Profiles of O_3, H_2O, and tracers (e.g. CH_4, N_2O)
temperature and wind fields
tropics and across the subtropics (all seasons)
high latitudes (winter)

- **What are the sources and distributions of tropospheric pollutants?**

Topic: Emissions from biomass burning, industry, and agriculture that result in high concentrations of O_3, NO, NO_2, HCHO, aerosols, etc... and the fate of O_3, NO_2 and aerosols in the tropical atmosphere
Rationale: The impact of pollutants on the nitrogen cycle, the global budget of NO_x and NO_x emissions, and the coupling between chemistry and transport in the tropical troposphere are not well known.
Measurements proposed: airborne *in situ* measurements of O_3, NO_2, and aerosols
assessing the size of the pollutant plumes
tropics, burning season

- **What are the roles of upper tropospheric water vapor, aerosols, and ozone in climate change?**

Topic: The role of water vapor in determining polar winter stratospheric temperatures
Rationale: Models predict additional ozone depletion due to an increase in atmospheric water vapor content
Measurements proposed: balloon *in situ* measurements of H_2O, O_3, NO_2
aerosols, PSCs, including particle size and composition
ground-based aerosol and ozone/temperature lidar
routine ozone sondes
high latitudes, winter

Three missions that are being developed to address the above topics are described in more detail in Appendix 7C. The Tropical Composition and Climate Coupling Experiment (TC^3, section 7.C.1) is a multi-year, multi-sensor deployment with two primary science goals. These are to define and understand the chemical boundary condition for the stratosphere with an emphasis on processes that affect ozone, and define and understand the response of the atmospheric hydrological cycle to climate change. Two missions focused on tropospheric chemistry are discussed in Appendix 7C.2. The first mission, the Intercontinental Chemical Transport Experiment (INTEX), is part of a larger program of aircraft missions aimed at quantifying the chemical outflow from northern midlatitude continents and the associated intercontinental transport of pollution. The second takes advantage of the Large-Scale Biosphere-Atmosphere Experiment in Amazonia (LBA), a US-Brazilian ground-based program focused on understanding the budgets of carbon, energy and water vapor in the Amazon Basin. The LBA Airborne Regional Source Experiment/Transport and Chemistry Experiment in Brazil (LARS/TRACE B) address the need to quantify the sources and sinks of environmentally important special in the Amazon Basis, and the implications of processes in the Amazon Basis for the global atmosphere. These two experiments share the common theme of quantifying the outflow of environmentally important species from major source regions to the atmosphere.

5.2.4 Aura Intercomparisons

Intercomparisons among the four Aura instruments will play a big role early in the mission, since there is significant overlap between the measurement suites and the locations of observations. The details of such comparisons need careful planning. The initial thrust will be on Level 2 coincidences and zonal mean comparisons to clarify the relative biases between common measurements. Comparisons of gridded products (Level 3) will await development of Level 3 outputs from all teams. A data assimilation system may be useful to identify biases in the Aura ozone data relative to that from different instruments, or to identify biases in the Aura ozone products relative to each other. Ultimately, for a constituent like ozone that is measured by several instruments, a data assimilation product could be developed that combines the best information from each Aura instrument into a definitive product. However, data assimilation is not possible without knowledge of uncertainties and relative biases between the various data sets.

5.2.5 The Use of Atmospheric Modeling and Other Methods for Validation

Models

Atmospheric models and climatological data sets can be used to test whether Aura measurements are reasonable. Model comparisons can be useful for noisy measurements and for cases where little climatological information exists, e.g. for stratospheric N_2O_5, OH, HO_2, BrO, HOCl, or for tropospheric NO_x and HNO_3. Monthly model values can easily be compared to averaged fields (for example, daily and monthly averages) as an initial consistency check.

More specific model comparisons that are initially focused on validation of data should occur within the Aura instrument teams and through collaborations between the teams and modeling groups. For example, assimilation techniques and techniques such as following parcel trajectories can compare different (non-coincident) data sets to each other. This was used successfully at a late stage in the evaluation of UARS data versus other data sets and to intercompare different UARS instrument results as described in the WMO/SPARC (1998) report on ozone trends. Such modeling efforts will undoubtedly be used earlier on during the Aura validation efforts. The OMI team anticipates use of assimilation techniques for meeting coincidence requirements necessary for validation. Assimilation techniques are already used for GOME O_3 validation. However, constituent assimilation requires full characterization of error statistics; such characterization cannot be completed prior to the validation activities.

Statistical Methods

Two-point statistics and Correlative Measurements

The differences between two measurements that are not exactly collocated in space or time or that have different resolution will include some measure of geophysical variability that is unrelated to the measurement error per se. Statistical estimates of this contribution and its dependence on scale can be made from existing high resolution aircraft and balloon data. This is a pre-launch activity that will provide quantitative estimates of the degree to which a point measurement is representative of a spatial average. These statistics will also provide coincidence criteria and will address the important issue of scale invariance, i.e. whether the statistics of variability on different scales has a simple relationship under a change of scale. Estimates of measurement uncertainties for the Aura instruments can be used together with the two-point statistics to provide guidelines for the design of correlative measurement campaigns by quantitatively estimating when and where the contribution from natural variability is likely to exceed differences due to measurement uncertainties.

Statistical Aura Intercomparisons

Comparisons of area-weighted PDFs (Probability Distribution Functions) of the Level 2 data can be made soon after launch. These distributions easily quantify the full range of variability at each vertical level and will identify biases as relative shifts in the peak of the distribution. This will identify problems with measurements in the tails of the distribution that can have a large effect on the mean, yet are easily undersampled. Two-point statistics, e.g. differences across a given vertical or horizontal scale, or point-to-point variability along the satellite track will quantify the scale-dependent variability as measured by each instrument and will be useful in interpreting differences between nearly coincident measurements taken with different Aura instruments.

5.3 Summary of Aura Plans for Post-Launch Activities

The following paragraphs summarize the plans for validation activities following Aura launch. Some of the specifics of this planning will have to await further definition of the investigations to be selected in support of Aura validation and science.

5.3.1 Aura Measurements and Validation Overview

Tables 5.10, 5.11, and 5.12 summarize the measurements needed for validation of stratospheric profiles, tropospheric profiles, and column densities and other needs, respectively. Expected satellite, ground-based, and sonde data sources and opportunities are listed generically (for more details, see Table 5.3), with columns for satellite and ground-based data indicating expected amounts and quality/extent of match with Aura data. A priority column (with 1 for high, 2 for medium, 3 for lower priority) is used to indicate correlative data need as well as scientific importance of the Aura measurements (based on section 5.2.3.2). More details for each product can be found in section 5.2.3.3.

Although a significant number of tropospheric chemistry campaigns have occurred in the 1990's, there are no global data bases for most tropospheric constituents. Validation activities for tropospheric data are necessary over a broad range of latitudes and seasons.

5.3.2 Aerosols and Clouds

Besides the scientific interest in aerosols and clouds, these particles can affect the retrievals of other Aura products in the lower stratosphere and troposphere. OMI is sensitive to light-absorbing lower tropospheric particles (desert dust, particles from fires); HIRDLS and TES will sense stratospheric sulfate, polar stratospheric cloud, and upper tropospheric cirrus particles; the MLS experiment senses large particles (larger than 100 μm). A key validation source for the OMI experiment will be the aerosol optical thickness and single scattering albedo values measured by the AERONET set of ground based instruments. The primary measurements desired for HIRDLS and TES are particle size measurements of sulfate, PSCs, and upper tropospheric cirrus, and lidar measurements of aerosol spatial distributions, as well as other satellite observations of the extinction of the three types of particles. Correlative tropospheric aerosol composition information would also be useful. For the MLS cloud ice and OMI cloud products, the primary validation will use data from the Earth System Science Pathfinder (ESSP) Project mission CloudSat and ESSP3 (formerly PICASSO-CENA), but for MLS campaigns including cloud measurements of large ice particles are desirable. Measurements of the composition of stratospheric PSCs would allow us to relate satellite spectral information to composition.

5.3.3 Column Densities

The most important**,** currently unmet, validation need for OMI column densities is for tropospheric NO_2 under polluted as well as clean conditions; tropospheric ozone column densities are also desirable, as part of Aura-related campaigns. Under polluted NO_2 conditions, column and profile information in the lower troposphere is essential for the column density validation. Choices for this validation requirement are currently limited.

The ozone column measurement, also high priority, can be validated by Brewer Dobson instruments, integrating sonde measurements or by comparison to other satellite measurements (i.e. TOMS, GOME, SCIAMACHY). Again, not many of these instruments are located in very polluted areas, thus additional measurements are needed.

An aircraft campaign (e.g., with a UV-VIS DOAS-type instrument aboard) in which measurements of tropospheric and stratospheric profiles and column densities of NO_2 and O_3 are performed, can be used for these purposes (see also 5.3.8 and 5.3.9).

Table 5.10. Aura stratospheric measurements and validation plans. Priorities (1, high; 2, medium; 3, lower) are for validation needs, with a consideration of scientific importance; a bracket indicates routine data are likely to provide significant/sufficient validation. *Correlative data sources and opportunities:* column **S** is for satellite data: ++ = sufficient/significant amount, + = moderate amount (some extra efforts may be needed), **-** = small amount or poorly matched (without extra efforts, proper validation cannot be performed); column **G** is for ground-based data, including sonde networks: "(C)" = column data with significant stratospheric contribution, "(c)" = column data of more marginal use for stratospheric validation. Column **B** (when filled in) represents a need/desire for balloon correlative data (X or D for existing capability or development needed); column **A** is for a similar need/desire for aircraft correlative data (lower stratosphere).

Parameter	**Priority**	**HIRDLS**	**MLS**	**TES**	**OMI**	**S**	**G**	**B**	**A**	**Comments**
Temperature	[1]	●	●	●		++	++	(X)	(X)	Sufficient correlative data (e.g., Op. Met., GPS, ARM data).
O_3	[1]	●	●	●	●	++	++	(X)	(X)	Campaign-derived horizontal gradients for profiles very desirable (lower strat.). Maintain existing ozonesonde programs.
H_2O	1	●	●	●		++	+	X	X	Campaign-derived horizontal gradients for profiles very desirable (lower strat.). Balloon profiles at range of latitudes are needed.
N_2O	1	●	●	●		++	-	X	X	Balloon profiles very desirable.
CH_4	1	●		●		++	-(c)	X	X	Balloon profiles very desirable.
HCl	1		●			-	-(C)	X	X	Balloon profiles very desirable.
OH	1		● $^{(*)}$			-	-(C)	X	X	Balloon profiles very desirable.
HNO_3	1	●	● $^{(*)}$	●		++	-	X	X	Balloon/aircraft data very desirable.
BrO	1		● $^{(**)}$			+	-(C)	X	X	Balloon profiles very desirable.
Aerosols, PSCs	1 (see comment)	●		●		++	+	X	X	In part for spectral information and retrieval needs. High need for aerosol data if large volcano erupts.
ClO	2		● $^{(*)}$			-	-	X	X	Balloon/aircraft profiles desirable (polar vortex also).
$ClONO_2$	2	●		● $^{(1)}$		++	-(C)	X	X	Balloon/aircraft profiles desirable (polar vortex also).
CFC-11, CFC-12	2	●				++	-(c)	X	X	Balloon/aircraft profiles desirable.
HOCl	2		● $^{(**)}$			-	-	X	X	Few correlative data. Balloon profiles desirable.
HO_2	2		● $^{(**)}$			-	-	X	X	Few correlative data. Balloon profiles desirable.
NO	2			●		-	-(c)	X	X	Balloon profiles (non-twilight data) desirable.
NO_2	2	●		●		++	-(c)	X	X	Balloon profiles (non-twilight data) desirable.
N_2O_5	2	●				+	-	X	X	Few correlative data. Balloon profiles desirable.
CO	2		● $^{(*)}$	●		++	-(c)	X	X	Some balloon profiles desirable (e.g., in polar vortex).
HCN	3		● $^{(*)}$			-	-(c)	X	X	Few correlative data. Balloon profiles desirable.
CH_3CN	3		● $^{(**)}$			-	-	X/D	X/D	Few correlative data.
SO_2 (volcanic)	3		● $^{(*)}$			+	-	(X)	(X)	Only important if stratospheric volcanic plume is generated.
Geopotential Hgt	[3]	●	●			++	++			

$^{(1)}$ Not a standard product, at least initially (requires more research). $^{(*)}$ This measurement often requires averaging. $^{(**)}$ This measurement always requires averaging.

Table 5.11. Aura tropospheric measurements (C_{trop} = tropospheric column density, with a validation need for profiles) and validation plans. Priorities (1, high; 2, medium; 3, lower) are for validation needs, with a consideration of scientific importance; a bracket indicates routine data are likely to provide significant/sufficient validation. *Correlative data sources and opportunities:* column **S** is for satellite data: ++ = sufficient/significant amount, + = moderate amount (some extra efforts may be needed), - = small amount or poorly matched (without extra efforts, proper validation cannot be performed); column **G** is for ground-based data, including sonde networks. Column **B** (when filled in) represents a need/desire for balloon correlative data (X or D for existing capability or development needed); column **A** is for a similar need/desire for aircraft correlative data (troposphere). Other balloon/aircraft needs are listed for the lower stratosphere in Table 5.10 (the Aura products below generally extend into the stratosphere).

Parameter	Priority	HIRDLS	MLS	TES	OMI	S	G	B	A	Comments
Temperature	[1]	● (2)	● (2)	●		++	++	X	X	Temperature data desirable in conjunction with other correlative tropospheric observations.
O_3	1	● (2)	● (2)	●	C_{trop} (1)	+	+	X	X	Campaign-derived horizontal gradients for profiles and tropospheric columns very desirable. Maintain existing ozonesonde programs.
H_2O	1	● (2)	● (2)	●		++	++	X	X	Campaign-derived horizontal gradients for profiles very desirable.
CO	1		● (2) (*)	●		+	+	X	X	Desirable to follow up on correlative data program similar to the one for MOPITT.
HNO_3	1			●		-	-	X	D	Few correlative data sources, none in lower troposphere; aircraft profiling very desirable.
NO	1			● (2)		+	-	X	X	Few correlative data. Diurnal effects are an issue.
NO_2	1			● (2)	C_{trop} (1)	+	-	X	X	Few correlative data. Diurnal effects are an issue. For OMI, tropospheric columns and profiles are needed for validating column densities in polluted regions.
Cloud properties	1	● (1)	● (1)	● (1)	●	+	-	X	X	In-situ data on cloud particle size distributions desirable. For OMI, the optical thickness of clouds, cloud albedo, & information about cloud system structure are desirable.
Cloud detection	[1]	●	●	● (1)	●	++	-			
Aerosols	1 (see comment)	● (2)		● (1)	●	+	+	X	X	Needed for aerosol product validation, but also for spectral information and other product retrieval needs. In-situ data on aerosol particle size distributions and composition desirable.
CH_4	2	● (2)		●		+	+	X	X	Desirable to follow up on correlative data program similar to the one for MOPITT.
HCN	2		● (2)			-	-	X	X	Few correlative data sources; profiles desirable.
N_2O	[2]	● (2)				-	++			Surface measurements adequate for troposphere.
CFC-11, CFC-12	[2]	● (2)				-	++			Surface measurements adequate for troposphere.
Geopotential Hgt	[3]	● (2)	● (2)			+	++			

(1) Not a standard product, at least initially (requires more research). (2) No measurement below the upper troposphere. (*) This measurement often requires averaging.

Table 5.12. Aura column density and other measurements (C = column density, C_{trop} = tropospheric column density) and validation plans. Priorities (1, high; 2, medium; 3, lower) are for validation needs, with a consideration of scientific importance; a bracket indicates routine data are likely to provide significant/sufficient validation. *Correlative data sources and opportunities:* column **S** is for satellite data: ++ = sufficient/significant amount, + = moderate amount (some extra efforts may be needed), **-** = small amount or poorly matched (without extra efforts, proper validation cannot be performed); column **G** is for ground-based data, including sonde networks. Column **B** (when filled in) represents a need/desire for balloon correlative data; column **A** is for a similar need/desire for aircraft correlative data (troposphere).

Parameter	Priority	OMI	TES	S	G	B	A	Comments
NO_2	1	C		+	+			Few correlative non-twilight ground-based data. Ground-based correlative data under polluted conditions needed, since troposphere dominates. Diurnal effects are an issue, see also Table 5.11.
NO_2 (tropospheric)	1	$C_{trop}^{(1)}$		+	-	X	X	Ground-based (or other) campaign correlative data under polluted conditions needed. Main satellite correlative data: SCIAMACHY (nadir-viewing mode).
O_3	[1]	C	$C^{(a)}$	++	+			Sufficient amount of ground-based correlative data expected, see also Table 5.11.
O_3 (tropospheric)	1	$C_{trop}^{(1)}$		+	+	X	X	Campaign efforts for validation of horizontal variability needed.
HCHO	2	C		+	-			Campaign efforts for ground-based column data needed (no routine ground-based correlative data sources). GOME also measures HCHO.
OClO	2	C		+	-			Few correlative non-twilight ground-based data. Diurnal effects are an issue.
BrO	2	C		+	-			Few correlative non-twilight ground-based data. Diurnal effects are an issue.
SO_2 (volcanic)	1	C	$C^{(1)}$	n/a	n/a			High priority if large volcanic eruption occurs.
SO_2 (background)	3	C	$C^{(1)}$	n/a	n/a			Under background conditions, no sensitivity, or high need for validation
UV fluxes, UV-B	2	•						Ground-based and airborne validation activities needed

(1) Not a standard product, at least initially (requires more research).

(a) Integrated column from TES profiles

5.3.4 Other Issues and Plans for Validation

There is a need for correlative surface albedo data (for OMI) and infrared surface emissivity (for TES). Raw radiance data from satellite instruments covering Aura wavelengths (e.g., GOME, SCIAMACHY, UARS MLS, ODIN/SMR, ASTER) can be used to perform consistency checks with Aura Level 1 data. The AES experiment will provide surface emissivity and near surface radiances for TES.

5.3.5 Ground-based Networks

Several ground-based networks (ozonesondes, Brewer/Dobson and Umkehr sites, radiosondes, NDSC, ARM, AERONET, and others) should provide accurate information about stratospheric and tropospheric profiles, and column densities for some of the constituents measured by Aura, as well as aerosol and cloud information (see Table 5.3). Such networks offer the best means for long-term validation of data from Aura and other satellites.

5.3.6 Other Satellite Data

Satellite measurements of stratospheric constituents expected during the Aura timeframe are given in Table 5.2 of this document. Observations that are validated prior to Aura launch will be useful for Aura validation. Data sets most likely to be useful for initial Aura validation studies will come from satellites launched ~2 years or more prior to Aura since the validation process, including reprocessing, can take years. Analyses of satellite-satellite comparisons can often point to certain problems beyond any systematic disagreements in absolute values.

Aura will follow Aqua by fifteen minutes in nearly the same orbit plane. The MLS instrument will make limb measurements 7.5 minutes behind the Aqua nadir point where AIRS and MODIS measure. This close formation will allow the water vapor measurements from AIRS and the cloud screening from MODIS to provide information for Aura instruments. Near the time of the Aura launch, the ESSP CloudSat and ESSP3 (PICASSO-CENA) missions will also be launched into the Aura/Aqua orbit plane; these satellites will follow Aqua by about 1 minute (and will be about 14 minutes ahead of Aura). The ESSP3 mission will make aerosol and cloud height measurements that will be especially useful to OMI and HIRDLS. In a similar fashion, measurements from other relevant correlative satellite programs should be exploited as much as possible.

5.3.7 Balloon Flights

Measurements of stratospheric profiles from balloon platforms are the only means to get high vertical resolution profiles for most constituents in the mid- to upper stratosphere (Table 5.10). A series of flights at 2 or more latitudes over a 2-3 year period is viewed as a minimum need. High latitude campaigns using balloons are needed to provide profiles under the perturbed conditions of polar winter/spring. In situ or emission data are preferable to occultation data for species with significant diurnal variation (and potential variation along the line-of-sight) such as NO and NO_2, for optimal comparison with the Aura measurements; clearly, coordination with Aura overpasses becomes even more important in these cases. Measurements of tropospheric profiles from balloon platforms are needed, especially for tropospheric and lower stratospheric NO_2 and ozone in polluted areas.

5.3.8 Campaigns

Campaigns involve coordinated deployment of aircraft, balloon and ground based platforms to address scientific questions concerning key issues in atmospheric chemistry and dynamics. Such campaigns to study stratospheric phenomena have been carried out since the mid-1980's. The instrument payload used in those campaigns has been made more complete, and now measures many quantities of stratospheric interest. These data, combined with satellite information, have been utilized to well characterize atmospheric phenomena. For example, winter polar expeditions (e.g., AAOE, AASE I, AASE II, SOLVE, THESEO) have made repeated measurements within and near the polar vortex. These data, combined with continuing ground based measurements in the polar region, suggest that while limited focused measurements in these regions are appropriate for validation, major campaigns need not be developed to recharacterize those regions. However, the tropical upper troposphere and lower stratosphere have not been so completely characterized as the winter polar stratosphere. Although field campaigns to measure tropospheric quantities have taken place in the 1990's, there are no global data bases for most tropospheric constituents. Validation activities for tropospheric data are necessary over a broad range of latitudes and seasons (see Section 5.2.3.1.3 and Table 5.4).

Such campaigns are being planned, with the additional requirement to fulfill specific Aura validation requirements. Themes being used to develop campaigns (section 5.2.3.5) have been identified in the context of the Aura scientific objectives (section 2) and the validation needs of Aura as presented in section 5. Descriptions of three missions are provided in Appendix 7C. The Tropical Composition and Climate Experiment (TC^3) is a multi-year, multi-sensor deployment with the goals of defining the chemical boundary condition for the stratosphere and the response of the atmospheric hydrological cycle to climate change. Two missions, the Intercontinental Chemical Transport Experiment (INTEX) and the Large-Scale Biosphere-Atmosphere Experiment in Amazonia focus on tropospheric chemistry issues. It is probably not possible to meet all the Aura needs of latitudinal and seasonal coverage for aircraft and balloon observations within the scope of these large campaigns.

5.3.9 Lower Stratospheric and Tropospheric Measurements for Aura Validation

Validation of Aura data in the lower stratosphere and troposphere is challenging. The validation strategy must take into account the geophysical variability of the region, large vertical gradients for constituents such as H_2O, O_3, CO, and limitations due to retrieval physics that reduce the precision of retrieved quantities. For some of the Aura products (ozone, water vapor up to ~ 150 hPa, and aerosols), ground-based networks provide sufficient data (in certain places) for statistical comparisons. Aircraft underflights of the satellite footprint can provide horizontal validation and scientific information that ground-based or balloon-borne measurements generally cannot. For limb measurements, coincidence between a satellite overpass and an aircraft flight is always limited because a satellite measurement is instantaneous compared with the several hours required for an aircraft to explore a satellite footprint. A high priority in exploration of the satellite footprint is the along-track gradient since this gradient has the greatest impact on the retrieval algorithm for limb measurements (ahead of or behind the satellite). For nadir-viewing instruments, with relatively small footprints, aircraft measurements have the additional advantage of providing many correlative measurements spaced closely together, which boosts the statistical robustness of the intercomparison and provides a handle on horizontal variability.

As discussed in sections 5.2.3 and 5.2.3.1.3, major tropospheric aircraft campaigns are limited in spatial and temporal coverage, and will probably not meet the requirements for TES validation summarized in Table 5.4. For the tropospheric observations that are the primary science products of TES, for the tropospheric and lower stratospheric observations from HIRDLS and MLS, and for the tropospheric column measurements of OMI, such campaigns will have to be supplemented by smaller, targeted aircraft campaigns that address remaining specific needs.

5.3.10 Models

After launch, fields from model simulations will be used for comparisons with measurements of all constituents, but especially for those measurements that are noisy and must be spatially and temporally averaged to have geophysical meaning. Assimilation techniques and techniques such as following parcel trajectories will also be utilized.

6 Data Archival and Data Exchange Issues

The data archival location for Aura products will be the NASA Goddard Space Flight Center (GSFC) Distributed Active Archive Center (DAAC). The data processing itself will be performed at various sites, depending on the specific Aura instrument.

For the purposes of validation and intercomparisons, exchange of data between investigators providing correlative data and the EOS Aura investigators will be required. It is expected that the GSFC DAAC or some other central location will serve as repository for the correlative data (non-satellite, because of the lower volumes of data) for Aura. Since different investigators, institutions, organizations, and/or countries are likely to have differing protocols or guidelines regarding data exchange and data formats (and regarding the use of data in publications), these issues will need to be dealt with in the not-too-distant future, possibly on a case-by-case basis.

More details will be discussed in a future revision (or second phase) of this document, after more inputs and plans have been developed.

7 Appendices

7.A Appendix A: Aura Instrument Measurement Techniques

7.A.1 HIRDLS Measurement Technique

The fundamental measurement in infrared limb scanning is atmospheric thermal emission as a function of the relative position of the line-of-sight of the instrument as it is scanned across the limb; measurement of thermal emission from satellites permits global coverage, both day and night (including the polar night). The vertical distribution of atmospheric quantities, such as temperature or ozone concentration, can be derived with high vertical resolution (e.g. $\leq$ 1-2 km) using this technique. Because of the combination of the limb geometry and the exponential fall off of density with altitude, most of the contribution to observed radiance arises from very near the tangent point. The limb weighting function is further broadened by the instrument field-of-view and therefore should be limited to 1-2 km at the limb. All the radiation reaching the instrument originates from atmospheric emission; contributions to the signal from the cold space background are negligible and therefore signal variations at the entrance aperture of the instrument are due only to variations in atmospheric emission. The significantly longer gas emission path along the limb results in a larger emission signal enabling measurement of more tenuous gas concentrations to higher altitudes. The upper altitude limit of vertical coverage is set when the signal-to-noise approaches unity. The lower altitude limit is determined by limb opacity, including the presence of thick aerosol or clouds.

During the data reduction process, the measured vertical profiles of the radiance emitted by CO_2 (which has a known distribution in the atmosphere) are inverted to determine the temperature of the atmosphere as a function of pressure. Limb observations in two or more spectral bands with differing optical properties located near the 15 μm band of CO_2 allow a self-consistent reference pressure to be found by requiring that the temperatures derived from both spectral channels be the same (Gille and House, 1971). The relative pressure levels between radiance samples are determined by knowing the relative line-of-sight angle between samples. The two-spectral channel technique of Gille and House alleviates the stringent requirements for absolute knowledge and control of spacecraft attitude and position. The temperature profile is therefore retrieved as a function of pressure. Subsequently, retrieved temperature profiles are combined with measured vertical profiles of radiance emitted by other gases or aerosols to determine their vertical distribution. Finally, regional and global maps of the temperature, and gas and aerosol concentrations can be constructed from the vertical profiles.

The High Resolution Dynamics Limb Sounder is an infrared limb-scanning radiometer designed to measure atmospheric limb emission in 21 narrow-band spectral channels operating at wavelengths in the range from 6 to 18 μm. A schematic diagram of the HIRDLS instrument is shown in Figure 7.1. The instrument consists of nine subsystems; the key subsystems are described below. The structural-thermal subsystem (STH) provides an outer cover to create a stable mechanical and thermal environment for the instrument, a radiator panel for removing heat from the mechanical cryocooler, and a baseplate on which the telescope subsystem is mounted. The instrument views rearward from the spacecraft with the boresight inclined approximately 25 degrees below the local horizon. The sunshield subsystem (SSH) includes a moveable door to prevent sunlight from directly illuminating the instrument aperture when the satellite is in the high latitude portion of the orbit.

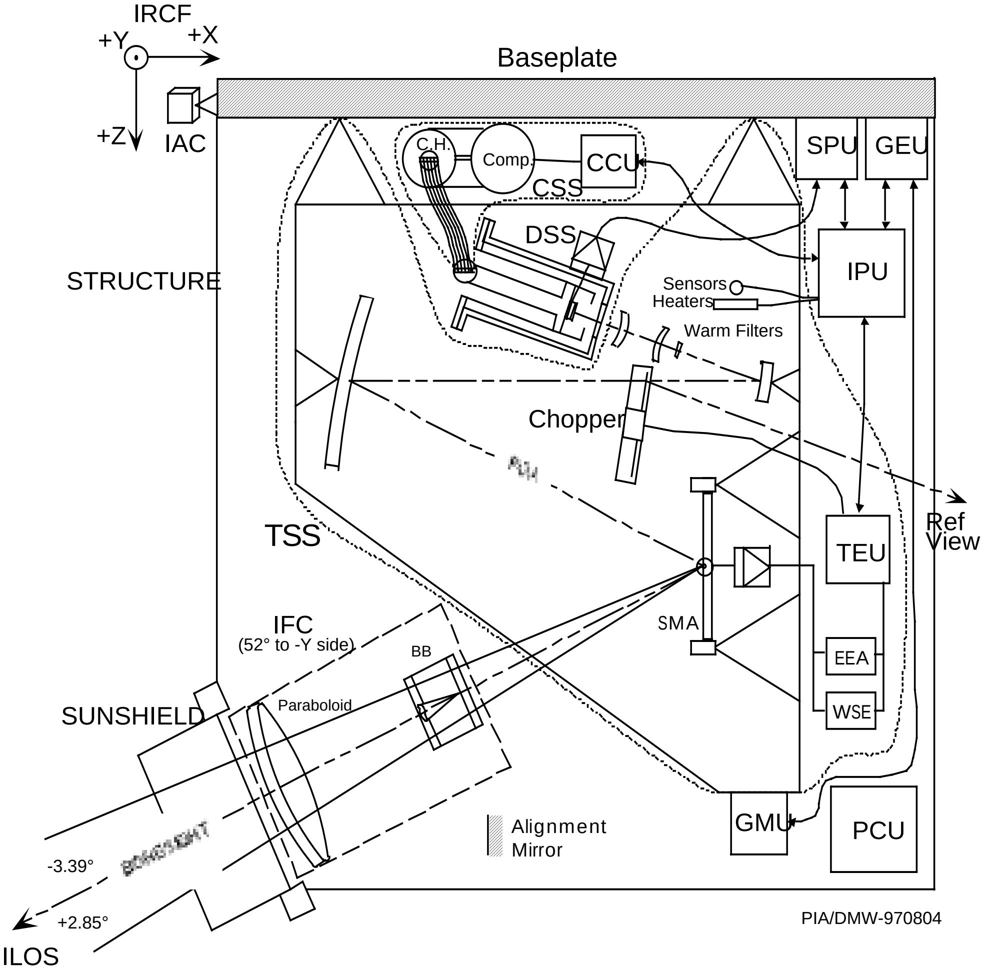


Figure 7.1. Schematic diagram of the HIRDLS instrument.

Limb radiation enters the instrument aperture and is collected by the optical telescope after reflection off the flat scan mirror. The telescope subsystem (TSS) consists of a two-axis scan mirror, an off-axis, 3-mirror Gregorian reflective telescope, and two Ge lenses to relay the image of the atmosphere produced by the telescope onto the focal plane consisting of 21 infrared detectors while maintaining good image quality. The optical system is designed to image a 1-km vertical dimension at the atmospheric limb a distance of 3000 km away onto detectors with a vertical dimension of 82 μm. The scan mirror (SMA) rotates about two axes to scan the instrument field-of-view in azimuth (over a 60° range) and elevation to view the desired part of the atmospheric limb or to view the collimated beam of a small, high quality blackbody for in-flight radiometric calibration (IFC). The blackbody is designed to have high emissivity, small thermal gradients and its temperature is precisely monitored by high quality platinum resistance thermometers. The calibration mirror temperature is controlled to within 1 K of the IFC blackbody temperature to minimize radiometric error due to uncertainty in the IFC mirror emissivity. The nominal calibration period is 66 seconds. This provides an end-to-end gain calibration point using the same optical configuration as used in limb measurements. A zero radiance calibration point is provided every 10 seconds by viewing cold space at the top of each vertical profile. Spectral selection is achieved through the use of 21 individual interference filters held at a fixed 301 K temperature and located at an intermediate focal plane. A second set of filters is located on the cold focal plane in close proximity to the detectors, having roughly twice the spectral bandpass of the warm filters. The cold filters are necessary to achieve a high level of out-of-band spectral blockage and to significantly reduce unwanted optical cross talk due to scattering by or internal reflections from the Ge lens relay system. The detector focal plane dimensions and the relative positions of the spectral channels are shown in Figure 7.2. The center detector column has been offset from the middle to allow room for electrical connections to be made. The alignment quad-cell detector at the top of the array is to facilitate pre-flight testing and will not be operational in-flight.

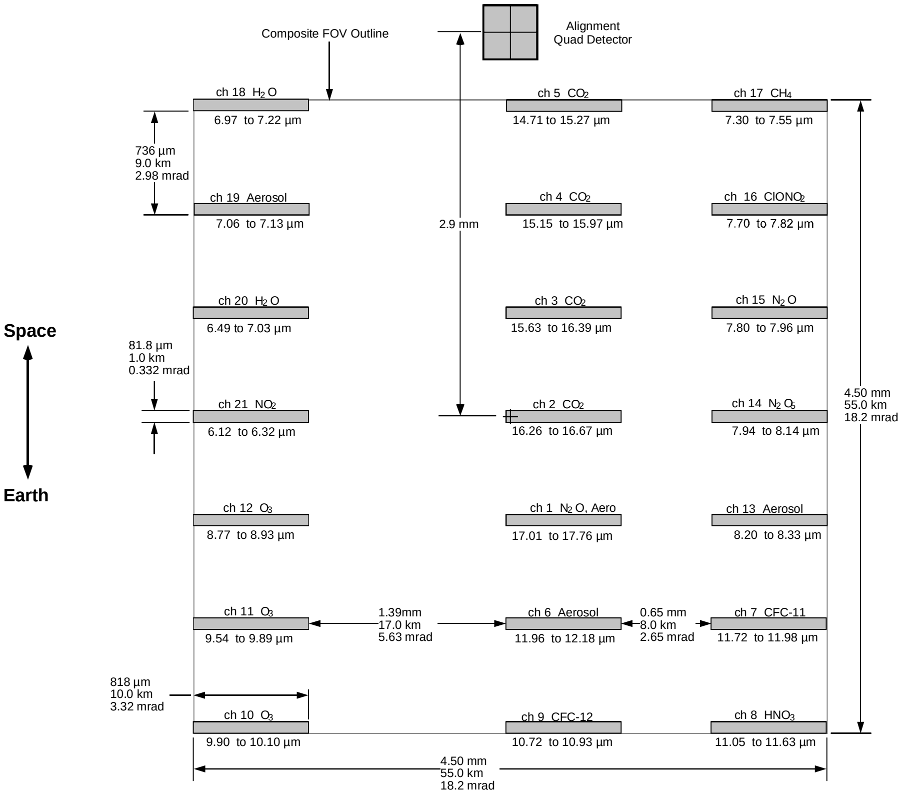


Figure 7.2. HIRDLS focal plane array.

The detector fields-of-view are alternately scanned upward and downward across the limb at a nominal scan rate of 0.32 deg/sec in the global observation mode. The angular position of the scan mirror relative to the optical bench is measured by optical encoders every 12 msec. Any inertial motion of the optical bench produced by spacecraft and instrumental disturbances will introduce undesired motion of the LOS, which will not be sensed by the encoders. It is expected that data from the spacecraft attitude control system will not be of sufficient precision nor will the relationship between the spacecraft gyro and HIRDLS line-of-sight be known precisely enough to meet this requirement. Therefore, a multi-axis gyroscope is mounted to the optical bench to measure bench motion relative to inertial space, making corrections to pointing knowledge possible. The gyroscope subsystem (GSS) consists of a mechanical unit, which is mounted directly to the optical bench providing angular motion measurements of the bench. The gyroscope unit is a GEC-Marconi Avionics Type 125 gyro with an electronic unit (GEU) specifically designed for HIRDLS requirements. Incoming atmospheric radiation, collected by the primary mirror, is mechanically chopped at a nominal frequency of 500 Hz by a reflective rotary chopper located at the first focal plane. The chopper reflects a view of space via a relay mirror to the detectors when closed. The radiant signal is detected by MCT detectors cooled by a

Stirling cycle cryocooler (the CSS) operating near 65 K and controlled by the cooler electronics unit (CEU). The detector subsystem consisting of the focal plane array and a second set of spectral blocking filters are housed in a vacuum dewar assembly (DSS). The detected signal is electronically filtered, demodulated by sampling the waveform synchronously with the chopping frequency and digitized (16-bit analog-to-digital converter). A programmable lowpass digital filter is applied; the signal samples are decimated by a factor of 6 to a final sampling rate of nominally 83.3 Hz before being output to the telemetry stream. The instrument control and onboard data processing functions are performed by a flexible on-board microprocessor, referred to as the instrument processing unit (IPU), which can be programmed from the ground. The IPU controls the GMU via a gyro electronics unit, and similarly the mechanical chopper and scan mirror commands through the telescope electronics unit (TEU).

7.A.2 MLS Measurement Technique

EOS MLS has heritage from a number of aircraft and balloon experiments, and especially from the MLS experiment on the Upper Atmosphere Research Satellite (UARS). Development of the MLS experiments began at the Jet Propulsion Laboratory in the mid-1970's and included instruments deployed on aircraft [e.g., Waters et al. 1979] and balloon [e.g., Waters et al. 1981] prior to application of the technique from space. The MLS instrument that was launched 12 September 1991 on UARS [e.g., Reber et al. 1993] is the first application of the microwave limb sounding technique from space. The instrument is described by Barath et al. [1993] and uses ambient-temperature double-sideband heterodyne radiometers that operate near 63 GHz, 183 GHz and 205 GHz. The primary data products for which UARS MLS was designed are stratospheric ClO, O_3, H_2O and atmospheric pressure at the tangent point of the observation path (to provide a vertical reference for the other measurements). Temperature is also obtained from the 63 GHz radiometer that provides the pressure measurement.

Microwave limb sounding obtains remote measurements of atmospheric parameters by observations of millimeter- and submillimeter-wavelength thermal emission (radiances) as the instrument field-of-view (FOV) is scanned through the atmospheric limb. The geometry is sketched in Figure 7.3.

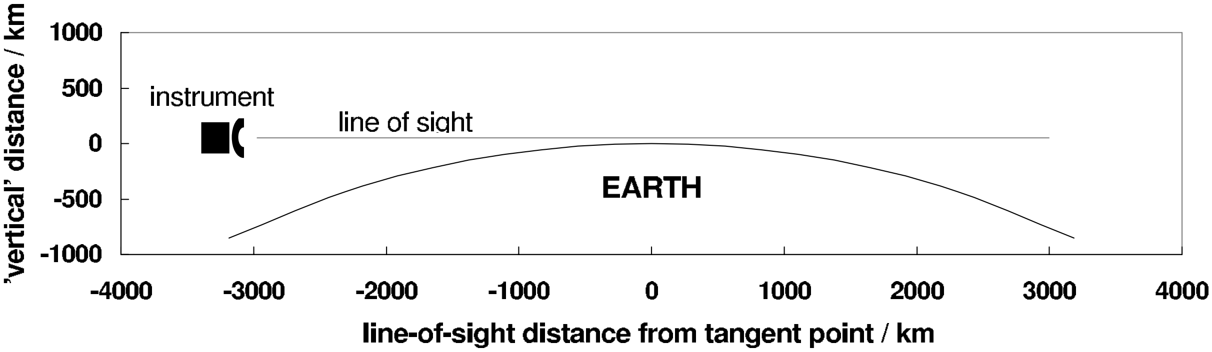


Figure 7.3. MLS measurement geometry, drawn to scale with an instrument in a 705 km altitude orbit (that of the Aura satellite) and the line of sight having 50 km tangent height. The size of the instrument is grossly exaggerated, of course. The orbit plane for EOS MLS is the plane of the paper.

Features of the technique, described further by Waters [1993] include:

- the ability to measure many atmospheric gases, with emission from molecular oxygen providing temperature and pressure;

- reliable measurements, even in the presence of heavy aerosol, cirrus or polar stratospheric clouds that degrade shorter-wavelength ultraviolet, visible and infrared techniques;
- the ability to make measurements at all times of day and night, and provide global coverage on a daily basis;
- the ability to spectrally resolve emission lines at all altitudes, which allows measurements of very weak lines in the presence of nearby strong ones and thus measurements of chemical species with very low atmospheric abundances;
- composition measurements that are relatively insensitive to uncertainties in atmospheric temperature;
- a very accurate spectral line data base [e.g., Pickett et al. 1992, Oh and Cohen 1994] [however better spectroscopic data are desired, see section 4.3.1.2];
- instrumentation that has very accurate and stable calibration. (For example, analyses of UARS MLS measured 'space radiances', indicate less than 0.02% change in antenna mirror reflectivity over a 5-year period in orbit. This implies an upper limit of 0.02% change in calibration due to mirror degradation, which is thought to be the largest contributor to calibration changes), and
- instrumentation that has adequate sensitivity, without necessarily requiring cooling, and good vertical resolution set by size of the antenna.

Having several spectral channels covering a single emission line (and resolving this line at all altitudes of interest) provides robust measurements, since geophysical quantities can be obtained from the channel-to-channel spectrally-varying component of the measured thermal emission. Extraneous effects, such as stray radiation, generally have spectrally-flat emission over the spectral range used for measurements, and their uncertainties do not usually have first-order effects on the retrievals of geophysical parameters. The widths of spectral lines in the millimeter and submillimeter wavelength spectral regions used by MLS are dominated by pressure (collisional) broadening throughout the troposphere and stratosphere, resulting in the linewidth being an approximately exponential function of height up to ~50-70 km. Doppler broadening dominates the linewidth at higher altitudes.

7.A.3 TES Measurement Technique

TES acquires high resolution infrared spectra of the naturally occurring infrared emission from the Earth's atmosphere. These spectra contain spectral features unique to the emitting species and from them the composition and state of the atmosphere are derived. The instrument is a Fourier Transform spectrometer that measures spectral radiance in the 650 - 3050 cm^{-1} (3.3 - 15.4 µm) spectral range with a resolution of 0.1 cm^{-1} (nadir viewing) or 0.025 cm^{-1} (limb viewing). Spectra with 0.1 cm^{-1} and 0.025 cm^{-1} resolution are acquired in 4 s and 16 s respectively. High spectral resolution and broad spectral coverage are essential for measuring the key atmospheric species over the 0 to 30 km altitude range that TES observes. It also allows a comprehensive survey of the entire suite of molecules found in the troposphere and lower stratosphere. The high spectral resolution minimizes detection interference between species and insures that high vertical resolution is maintained over the observed altitude range.

Both limb and nadir observation modes are essential. Many of the spectral features that TES observes are very weak (especially the nitrogen oxides) and limb-viewing markedly enhances their measurability (with the deficiency that cloud interference is much more likely than in nadir viewing). In contrast, due to high water opacity in the lower troposphere, many lower tropospheric species are only measurable with nadir views.

In order to improve signal-to-noise ratio and collection efficiency, TES is radiatively cooled to ~180K. In addition, the observational spectral range is divided into 4 sub-regions, each observed with a separate co-aligned 1x16 array of independent detectors actively cooled to 65K. The detectors are HgCdTe operated in the photovoltaic mode. The optical bandwidth of each spectral sub-region is further restricted to ~250 cm^{-1} by interchangeable filters. The spectral ranges of the filters are listed in Table 7.1.

Table 7.1. TES bandpass filter spectral ranges.

Array	**Filter**	**Spectral Range (cm^{-1})**	**Spectral Range (μm)**
1A		1900 - 3050	3.279 - 5.263
	1	1900 - 2250	4.444 - 5.263
	2	2200 - 2450	4.082 - 4.545
	3	2425 - 2650	3.774 - 4.124
	4	2600 - 2850	3.509 - 3.846
	5	2800 - 3050	3.279 - 3.571
2A		1100 - 1950	5.128 - 9.091
	1	1100 - 1325	7.547 - 9.091
	2	1300 - 1550	6.452 - 7.692
	3	1500 - 1750	5.714 - 6.667
	4	1700 - 1950	5.128 - 5.882
1B		820 - 1150	8.696 - 12.20
	1	820 - 1050	9.524 - 12.20
	2	950 - 1150	8.696 - 10.53
2B		650 - 900	11.11 - 15.38
	1	650 - 900	11.11 - 15.38

7.A.4 OMI Measurement Technique

The OMI instrument has been developed in the Netherlands by Fokker Space B.V. and TNO-TPD, in cooperation with Finnish industrial partners (Patria Finavitec Oy Systems and VTT Automation) and EEV in England. The Netherlands Agency for Aerospace Programs (NIVR) and the Finnish Meteorological Institute (FMI) manage the development with funding from each country for its part.

OMI is a nadir-viewing instrument, measuring the Sun's irradiance and the radiance scattered back by the Earth's atmosphere. It is designed as a compact UV/visible imaging spectrograph, using two-dimensional CCDs for simultaneous spatial and spectral registration [Levelt et al., 2000a, De Vries et al., 2000, Laan et al., 2000, Stammes et al., 1999, Smorenburg et al., 1999]. It measures the spectral range 270-500 nm, in order to cover the UV and visible absorption bands of O_3, NO_2, BrO and SO_2, and to retrieve aerosols, cloud cover, and cloud pressure. This is achieved with two channels: a UV-channel with full performance range 270-365 nm, and a visible channel with full performance range 365-500 nm; here 365 nm is the 50% sensitivity point of both channels. The UV and visible channels overlap between 350 and 380 nm. Within the UV channels the straylight could exceed the radiance at the shorter wavelengths. The intensity of backscattered radiance at higher UV wavelengths is normally three orders of magnitude higher than at shorter wavelengths. Therefore, straylight is suppressed by splitting the UV channel into two parts: UV-1 from 270 to 310 nm, and UV-2 from 310 to 365 nm.

A schematic overview of the instrument is given in Figure 7.4. Light enters the instrument via a wide field telescope, passes a polarization scrambler and is separated into UV and VIS parts by means of a dichroic mirror. In each of the two channels dispersion takes place by means of a grating. Each channel has a two-dimensional CCD as a detector. The spectrum is mapped along one direction of the CCD and the swath of 114° wide is mapped along the other direction. The CCD data are binned, A/D converted, and co-added in the Electronic Unit. The science and housekeeping data are sent to the spacecraft via the Spacecraft Interface. The optical bench as well as both CCDs are passively cooled to a temperature of 263 K. The total mass of the instrument is about 65 kg and the estimated average power needed is 65 W. The spectral characteristics of OMI are summarized in Table 7.2 below

Table 7.2. Spectral characteristics of OMI. "Resolution" means the FWHM of the slit function of 263 K.

Channel	Wavelength range	Resolution / sampling (nm)	Products
UV-1	270 – 310 nm	~0.42 (0.32)	O_3 profile, SO_2 (stratospheric)
UV-2	310 – 365 nm	0.45 (0.15)	O_3 column density and profile, SO_2, BrO, HCHO, clouds, aerosol
VIS	365 – 500 nm	0.63 (0.21)	O_3 column density and profile, NO_2 column density, clouds, aerosol, OClO

The fundamental OMI measurement is a nadir-viewed spectrum (270-500 nm) on a ground pixel 13 x 24 km^2. As the light captured is almost entirely sunlight that has been scattered either from the Earth's surface or in the atmosphere, the spectrum contains modulation features characteristic of the absorption and scattering cross-sections of the constituents of the atmosphere.

Algorithms are being developed and optimized to extract the column densities of such constituents as ozone, SO_2, BrO, and NO_2. More sophisticated algorithms are being developed to estimate vertical profiles, UV-B exposure, cloud pressure and cloud cover fraction, aerosol indices, and column densities of trace species like OClO and HCHO.

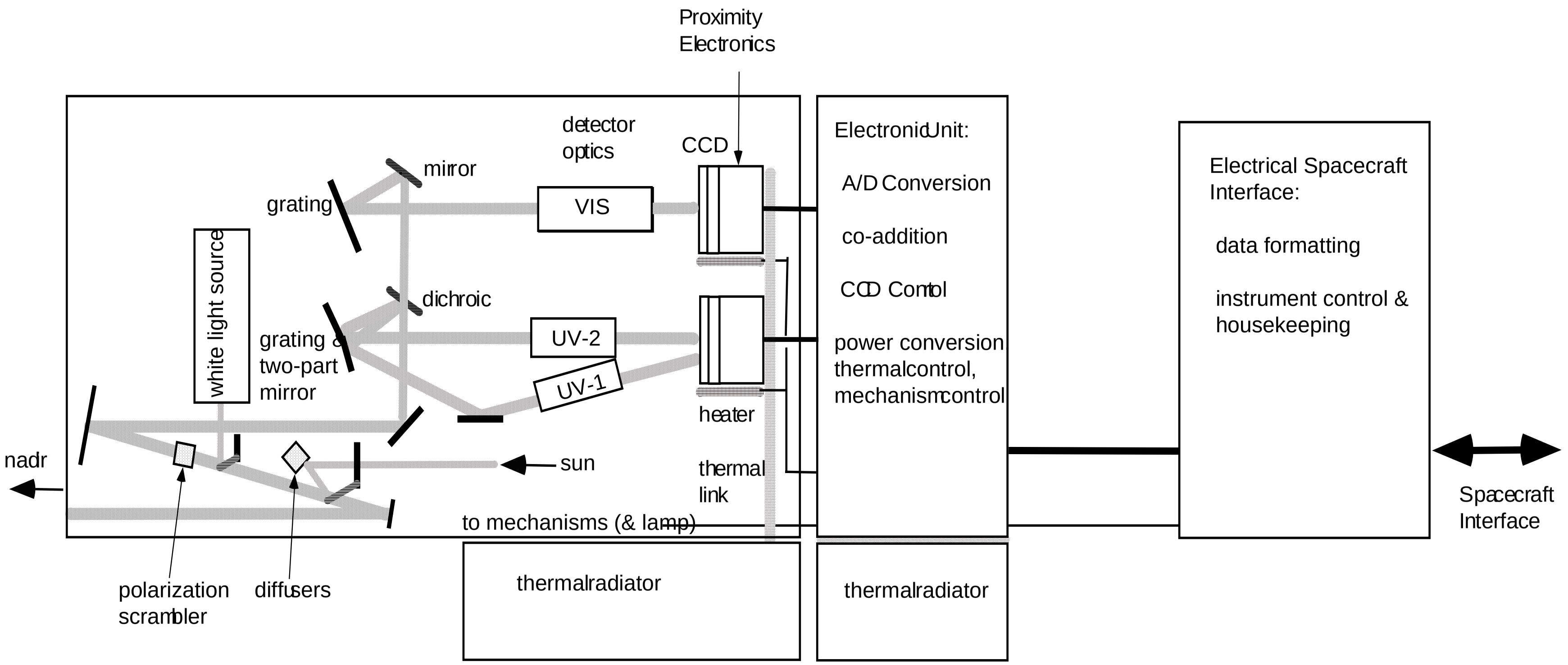


Figure 7.4. Conceptual design of OMI.

7.B Appendix B: Summary Information for other Satellite Instruments

The following is a summary list (arranged alphabetically by satellite or instrument name) of satellite-based instruments of primary interest to Aura investigators for validation purposes (see atmospheric products listed below), with some web-based references to be accessed for more information (along with the EOS Reference Handbook). We list here primarily the missions/instruments with launch dates prior to (or very close to) the planned Aura (mid-2003) launch date.

ADEOS-II (Advanced Earth Observation Satellite-II)

Instruments: include **ILAS-II** (Improved Limb Atmospheric Spectrometer-II), a solar occultation visible/infrared instrument, **AMSR** (Advanced Microwave Scanning Radiometer from Japan's NASDA – see also Aqua payload), **POLDER** (Polarization and Directionality of the Earth's Reflectance), a multi-channel (several channels between 443 and 865 nm), multi-angle optical sensor of reflected visible and near-infrared light at different polarizations.
Products: For ILAS-II, the products include temperature, O_3, HNO_3, CH_4, N_2O, H_2O, CFC-11, CFC-12, $ClONO_2$, and aerosols (with N_2O_5 also a possibility). For POLDER, aerosol optical thickness and water vapor content (column) are the products of most use for Aura product validation.
Orbital characteristics: Polar sun-synchronous, 803 km orbit, 10:30 a.m. descending node.
Coverage: Mainly polar latitudes, for ILAS-II occultation profiles. POLDER has global coverage.
Resolution: About 1 km (vertical) for ILAS-II.
Reference: http://www.eorc.nasda.go.jp/ADEOS-II/, and http://www-ilas2.nies.go.jp/ (for ILAS-II).

AMSU: see AIRS/AMSU/HSB description below (under Aqua).

Aqua satellite

Instruments: include **AIRS/AMSU/HSB** (Atmospheric Infrared Sounder/Advanced Microwave Sounding Unit/Humidity Sounder for Brazil), for infrared and microwave nadir soundings, **CERES** (Clouds and the Earth's Radiant Energy System, see the Terra payload)**,** and **AMSR-E** (Advanced Microwave Scanning Radiometer), a passive microwave radiometer.
Products: AIRS measures primarily temperature and humidity (troposphere), and ozone. AMSU is a passive microwave instrument, nadir-viewing (with cross-track scans to ± 48° from nadir); AMSU-A and AMSU-B (similar to HSB) use different frequencies (15 channels for AMSU-A, 5 channels for AMSU-B), with AMSU-A providing mainly temperature information, and AMSU-B humidity information. AMSR-E is less synergistic with Aura and focuses on land/ocean properties along with rainfall.
Orbital characteristics: Same 705 km orbit as Aura (polar, 98.2 degree inclination, sun-synchronous), but with 1:30 p.m. (ascending) node.
Coverage: Global.
Resolution: 1 to 2 km (vertical) and 13 km (horizontal), with 1600 km swath width for AIRS. For the microwave instruments, ~3 km in vertical, ~50 km horizontal field-of-view.
References: http://www-airs.jpl.nasa.gov,for AIRS; see also http://www2.ncdc.noaa.gov/docs/klm/**,** May 1999 User's guide for NOAA KLM System (including AMSU instruments).
http://asd-www.larc.nasa.gov/ceres/ASDceres.html for CERES;
http://wwwghcc.msfc.nasa.gov/AMSR/ for AMSR-E.

CloudSat satellite, will fly in formation with (1 minute behind) ESSP3 (PICASSO-CENA), so the radar footprint will overlap the lidar footprint.

Instruments: The primary instrument is **CPR** (Cloud Profiling Radar, operating at 94 GHz).

Products: Cloud-layer thickness, cloud base, cloud top height, cloud optical thickness, cloud water and ice contents.

Orbital characteristics: Essentially the same as Aura (and Aqua), but with a 1:31 p.m. node.

Coverage: Nadir-views along the orbit tracks (but no information between orbit tracks).

Resolution: The radar has ~1.4km footprint, to be averaged to produce 4 km along-track and 1.4 km cross-track data. Vertical resolution will vary (different modes) between 500m (normal mode) and 250m.

References: http://cloudsat.atmos.colostate.edu/

ENVISAT satellite

Instruments: 10 instruments, including **GOMOS** (Global Ozone Monitoring by Occultation of Stars), a UV/Visible (stellar) occultation sounder, **MIPAS** (Michelsen Interferometer for Passive Atmospheric Sounding), a Fourier Transform spectrometer for limb emission measurements, **SCIAMACHY** (the Scanning Imaging Absorption Spectrometer for Atmospheric Cartography), with heritage from GOME (but extending its UV/Visible range to the near infrared – observing scattered sunlight in nadir and limb views, and obtaining solar/lunar occultations as well); other ENVISAT instruments with some synergy with Aura include **MERIS** (Medium Resolution Imaging Spectrometer), a nadir-viewer targeting mainly the visible (reflected) spectrum for ocean color information (with some information on cloud top height, water vapor column, and aerosol load), **AATSR** (Advanced Along Track Scanning Radiometer), a two-view visible/infrared emission sounder, primarily targeting surface temperature and vegetation index data (with some cloud cover and cloud top height information), and **MWR** (Microwave Radiometer), for nadir measurements of integrated water vapor column and cloud liquid water content.

Products: For stratospheric constituents, GOMOS will measure primarily O_3, NO_2, NO_3, H_2O, and aerosols (with best sensitivity for nighttime data). MIPAS will measure O_3, H_2O, CH_4, N_2O, HNO_3, NO, NO_2, N_2O_5, $ClONO_2$, CFC-11, CFC-12, CFC-22, and CO profiles. SCIAMACHY will also measure a large suite of species, including profiles of O_3, CO, N_2O, NO_2, CH_4, H_2O, and aerosol extinction, stratospheric column information for HF, BrO, OClO, ClO, and tropospheric columns for HCHO, SO_2, and NO_3.

Orbital characteristics: polar, sun-synchronous, with a 10 a.m. descending equatorial crossing time.

Coverage: Global daily for atmospheric chemistry sounders (but not daily for some high resolution imagers).

Resolution: Varies (typically 2 to 3 km vertical resolution for atmospheric constituents).

References: http://envisat.estec.eas.nl/

ERS-2 (European Remote Sensing Satellite-2) [launched in April 1995]

Instruments: include **GOME** (Global Ozone Measurement Experiment), a UV/Visible/near-IR nadir viewing spectrometer, and **ATSR-2** (Along-Track Scanning Radiometer), a nadir along-track scanner at UV, IR, and microwave channels.

Products: GOME produces O_3 (profile and column), and mostly column information about H_2O, HCHO, NO, NO_2, ClO, OClO, BrO, and SO_2. ATSR-2 gives cloud top temperature/height, cloud cover, aerosol amounts (tropospheric), tropospheric H_2O and liquid water content (+ surface temperature, vegetation).

Orbital characteristics: polar, sun-synchronous.

Coverage: Global coverage in 3 days.
Resolution: GOME has 960 km swath, with 320x40 km spatial resolution, vertical resolution of 6 km in troposphere, 4 km in stratosphere. ATSR-2 has swath width of 500 km, with 1 to 20 km field of view resolution.
References: For GOME, see e.g. http://www.iup.physik.uni-bremen.de/ifepage/gome.html

ESSP3 (formerly PICASSO-CENA) mission, Pathfinder Instruments For Cloud And Aerosol Spaceborne Observations-Climatologie Etendue des Nuages et des Aerosols, will fly in formation with (1 minute ahead of) CloudSat, so the radar footprint will overlap the lidar footprint.
Instruments: The primary instrument planned for this mission is the lidar (532 nm and 1064 nm polarization sensitive lidar, for vertical profiles of thin clouds and aerosols); other plans include an infrared imager (to combine with lidar for retrievals of cirrus particle size) and a wide field camera.
Products: Aerosol and cloud height/thickness, aerosol and cloud extinction and optical depth, cloud ice/water phase information; also cloud emissivity, and cirrus effective particle size.
Orbital characteristics: Essentially the same as Aura (and Aqua), but with a 1:30 p.m. node.
Coverage: Nadir-views along the orbit tracks (but no information between orbit tracks).
Resolution: Lidar has ~88m footprint (oversamples CPR footprint).
References: http://www-essp3.larc.nasa.gov/picasso.html .

GPS (Global Positioning System)
Instruments: the system consists of a constellation of microsatellites, with 24 radio transmitters in 12 hr orbits (at ~26,000 km), with receivers (all on microsatellites) in orbit (at ~600 km), allowing about 500 occultations per day; the goal is to increase the number of receivers from 2 (currently) to eight or more, to allow for several thousand profiles per day across the globe (in about the 2004 timeframe).
Products: temperature (from about 50 km down to upper troposphere, i.e. about 250K level, maybe almost to surface in dry polar regions), with high precision (0.3 K). Also H_2O (0.2 gm/kg precision if know temperature to better than 1.5 K), from about 1 to 8 km, and geopotential height (~ 10 m precision in lower stratosphere) for vertical range similar to temperature retrieval range.
Orbital characteristics: see above (distribution of orbits)
Coverage: global (eventually, coverage may be better than that from radiosondes, especially in the southern hemisphere)
Resolution: sub-km in vertical, a few hundred km in horizontal.
References: http://cosmic.cosmic.ucar.edu/ ; also http://www.ssc.se/ssd/msat/ace/ace.html

ICESat (Ice, Cloud and land Elevation Satellite)/GLAS (Geoscience Laser Altimeter System)
Instrument: GLAS is a facility laser instrument designed to operate in the near-infrared (1064 nm) and in green light (at 532 nm), to study topography and ice sheet changes, as well as clouds and aerosols.
Products: Of interest for Aura validation, cloud heights and aerosol and PSC profiles (of extinction, optical depth).
Orbital characteristics: near polar (94 degree inclination), 600 km altitude.
Coverage: Mainly narrow, along-track coverage.
Resolution: About 100m vertical resolution.
References: http://icesat.gsfc.nasa.gov/

METOP satellites

The MetOp (Meteorological Operational) satellite missions are a joint venture between ESA, EUMETSAT, NOAA, and CNES to provide the next-generation polar-orbiting weather satellites, starting in late 2003 or 2004.

Instruments: The array of instruments includes **AVHRR/3** (Advanced Very High Resolution Radiometer), **HIRS/4** (High Resolution Infrared Radiation Sounder), **AMSU-A** (Advanced Microwave Sounding Unit), **MHS** (Microwave Humidity Sounder), IASI (Infrared Atmospheric Sounding Interferometer), **GRAS** (Global Navigation Satellite System Receiver for Atmospheric Sounding), **ASCAT** (Advanced Scatterometer), and **GOME-2** (Global Ozone Experiment-2).

Products: Similar to current/previous NOAA products: temperature, humidity, clouds, ozone and other constituents.

Orbital characteristics: 9:30 a.m. equatorial (descending) crossing time.

Coverage: Global.

Resolution: Varies with instrument.

References: http://earth.esa.int/METOP.html

See also http://www.ncdc.noaa.gov/ol/satellite/satelliteresourcesabout.html

See also http://www.saa.noaa.gov/GUIDE/instrument_documents/

ODIN satellite

Instruments: SMR (Submillimetre Radiometer), and **OSIRIS** (Optical Spectrograph and Infrared Imaging System) [launched in Feb., 2001]. Uses the entire satellite motion for scanning the limb.

Products: For SMR, temperature, O_3, CO, N_2O, NO, NO_2, HNO_3, ClO, H_2O, HO_2. For OSIRIS, column and profiles for O_3, NO_2, NO (mesosphere), and aerosols.

Orbital characteristics: polar, sunsynchronous, with ascending node at 6:00 p.m.

Coverage: Global, but observation time is shared with astronomical observations (roughly half the days are reserved for Earth atmospheric observations).

Resolution: A few km (vertical), a few hundred km (horizontal).

References: http://www.ssc.se/ssd/ssat/odin.html

POAM III (Polar Ozone and Aerosol Measurement experiment on SPOT-4, Système pour l’Observation de la Terre) [launched in March, 1998]

Instrument: Solar occultation technique in UV/Visible/near-IR.

Products: Stratospheric profiles of O_3, H_2O, NO_2, aerosol (and PSC) extinction and temperature.

Coverage: polar latitudes (typically 14 profiles daily at 55N to 71N and 14 profiles at 63S to 88S).

Resolution: about 1 km in vertical.

References: http://opt.nrl.navy.mil/POAM/poam3/poam3.html

SAGE III (Stratospheric Aerosol and Gas Experiment), to be launched with the Meteor-3M platform and the International Space Station platform (at a later date).

Instrument: UV/Visible/near-IR grating spectroradiometer, for solar and lunar occultations.

Products: Stratospheric profiles (mainly) of O_3, H_2O, NO_2, NO_3, OClO; also aerosol extinction and cloud presence information.

Coverage: global (coverage improved over SAGE II because of lunar occultations), but the (more robust) solar occultations will provide only high latitude coverage for the planned Meteor platform orbit.

Resolution: 0.5 km in vertical.

References: http://www-sage3.larc.nasa.gov/

SBUV/2 (Solar Backscatter UltraViolet/2), on a series of NOAA satellites (following the SBUV 1978-1987 mission).
Instrument: Nadir-viewing monochromator observing scattered sunlight in the 200 to 400 nm wavelength range.
Products: Stratospheric O_3 profiles (25 to 55 km) and total column densities.
Coverage: global (daytime data).
Resolution: About 8 km vertical resolution; footprint is about 200 x 200 km.
References: (To be updated).

SciSat-1 satellite, ACE (Atmospheric Chemistry Experiment)
Instruments: ACE-FTS (Fourier Transform Spectrometer), and **MAESTRO** (Measurements of Aerosol Extinction in the Stratosphere and Troposphere retrieved by Occultation), both providing occultation profiles of upper atmospheric composition.
Products: ACE can measure all of the Aura stratospheric constituent profiles, except for radicals BrO, ClO, OH, HO_2, OClO. MAESTRO should add synergistic aerosol information.
Coverage: 30 occultations per day, limited latitude coverage (but closer to global coverage over a month timeframe).
Resolution: About 1 km (vertical resolution).
References: http://www.science.sp-agency.ca/J3-SCISAT-1.htm

SSM/T2 (Special Sensor Microwave Water Vapor Profiler)
Instrument: SSM/T2 instruments are part of the U.S. Defense Meteorological Satellite Program (DMSP). SSM/T2 is a cross-track scanning five channel (183 GHz) microwave sounder; measurements started in 1991 (archive at NOAA's National Geophysical Data Center).
Products: Water vapor at 3 levels in the troposphere.
Orbital characteristics: polar, sun-synchronous.
Coverage: Global.
Resolution: 3 levels in troposphere (low, mid, upper troposphere). Swath width of 1500 km; 28 observations (profiles) with 48 km resolution across the swath.
References: http://www.saa.noaa.gov/GUIDE/instrument_documents/ssmt2-sensor.html

Terra satellite [launched in Dec. 1999]
Instruments: MOPITT (Measurements Of Pollution In The Troposphere), an IR nadir viewing gas filter radiometer of primary relevance to Aura/TES data, **MODIS** (Moderate Resolution Imaging Spectroradiometer), an IR cross-track scanner, **MISR** (Multi-angle Imaging SpectroRadiometer), with 9 simultaneous camera views of the Earth at 4 wavelengths, **CERES** (Clouds and the Earth's Radiant Energy System), and **ASTER** (Advanced Spaceborne Thermal Emission and Reflection Radiometer), a visible to thermal infrared high-resolution (sub-100 meter) imager.
Products: CO columns (and troposphere layer amounts) and CH_4 columns for MOPITT. MODIS products include cloud properties (top pressure, coverage, thickness), and (column-integrated) aerosol properties (+ land/ocean surface properties). MISR products focus on cloud and (mainly tropospheric) aerosol properties. CERES products are mainly radiative fluxes, with some information about cloud properties and liquid water path. ASTER measurements focus on surface (emissivity, temperature) data, along with cloud information.
Orbital characteristics: polar, sun-synchronous, 10:30 a.m. (descending) equatorial crossing time.
Coverage: Global (but not daily for all instruments).

Resolution: For MOPITT, about 3 km (for tropospheric CO) in the vertical, and about 20 km spatial resolution.
References: http://eos-am.gsfc.nasa.gov/instruments.html

TIMED (Thermosphere, Ionosphere, Mesosphere, Energetics and Dynamics) **satellite**
Instruments: 4 instruments, including **SABER** (Sounding of the Atmosphere using Broadband Emission Radiometry), a multi-spectral radiometer measuring infrared limb emission.
Products: SABER measures mainly O_3 (10-100 km), H_2O (10 – 80 km), NO (90 – 180 km), and CO_2 (85 – 150 km).
Orbital characteristics: High inclination (but non-polar or sun-synchronous) orbit.
Coverage: Switches with period of about 2 months between mainly north (about 50S to 80N) and mainly south (about 80S to 50N).
Resolution: About 2 km (vertical), and a few hundred km (horizontal).
References: http://www.timed.jhuapl.edu/home.html

TOMS (Total Ozone Mapping Spectrometer)
Instruments: EP-TOMS or Earth Probe TOMS, and **QuickTOMS** versions should be available during the Aura timeframe (high synergy with OMI measurements). These instruments are cross-scanning backscatter UV (six-wavelength) sounders.
Products: Column ozone, column SO_2, aerosol optical depth / index, and UV reflectivity.
Orbital characteristics: Polar sun-synchronous (mid-morning equatorial descending crossing time).
Coverage: Global daily (or nearly so).
Resolution: About 40 km footprint.
References: http://toms.gsfc.nasa.gov/

Triana satellite
Instruments: Include a camera/imager at UV to near-IR wavelengths (**EPIC**, Earth Polychromatic Imaging Camera), a cavity radiometer (**NISTAR**, National Institute of Standards and Technology Advanced Radiometer), for data on Earth’s emitted radiant power, and a plasma-magnetometer.
Products: Ozone column and aerosol optical thickness; cloud height/emissivity; precipitable water; volcanic SO_2 column; UV radiance.
Orbital characteristics: Lissajous orbit at L1 (neutral point on Earth-sun line).
Coverage: Global and continuous coverage of the sunlit face of the Earth.
Resolution: 8 – 16 km.
References: http://triana.gsfc.nasa.gov/home/ and http://toms.gsfc.nasa.gov/

UARS (Upper Atmosphere Research Satellite) [launched in Sep. 1991]
Instruments: include **HALOE** (Halogen Occultation Experiment, IR solar occultation sounder), **MLS** (Microwave Limb Sounder), but may not be gathering data in the Aura timeframe.
The primary instruments that may provide atmospheric constituent data in the Aura timeframe are HALOE (still operational), a solar occultation infrared instrument, and MLS (mostly off during past year, but capable of obtaining measurements), a microwave limb sounder sensing thermal emission. Because of limited power availability (and data transmission and other issues), poorer data coverage now exists than earlier during the UARS mission.
Products: HALOE provides profiles for (mostly stratospheric) O_3, H_2O, HCl, HF, CH_4, NO, NO_2, and aerosols. MLS can provide stratospheric O_3, ClO, HNO_3, CH_3CN, and upper tropospheric humidity (other capabilities are now defunct because of failure or power-sharing constraints).

Orbital characteristics: 57 degree inclination precessing orbit, sweeping through local times every 36 days.

Coverage: HALOE occultations cover narrow latitude bands daily and sweep through latitudes roughly once per month. MLS coverage is nearly global on a daily basis (under best operational scenario), alternating north (about 35S to 80N) and south (about 80S to 35N) every 36 days on average.

Resolution: ~2 km for HALOE, and ~3 km for MLS vertical resolution.

References: See http://haloedata.larc.nasa.gov/home.html and http://www.mls.nasa.gov .

7.C Proposed Field Campaigns

7.C.1 TC^3: Tropical Composition and Climate Coupling Experiment

Science Goals:

- To define and understand the chemical boundary condition for the stratosphere with an emphasis on processes that affect ozone:
    1. *What are the physical mechanisms that control the humidity of the stratosphere?*
    2. *What is the fate of short-lived compounds transported into the upper tropical troposphere?*
- Define and understand the response of the atmospheric hydrological cycle to climate change:
    3. *What mechanisms maintain the humidity of the tropical and subtropical upper troposphere?*

7.C.1.1 Aura Yield and TC^3 Experiment Design

Table 7.1. TC^3 and satellite observations.

Observation	**Aircraft / Balloon**		**Spaceborne***	Science Goals
H_2O (Note *A*)	X / **D**	X	HIRDLS, MLS, TES, MIPAS, SCIAMACHY	1, 2, 3
HDO, $H_2{}^{18}O$ (Note *A*)			TES, SCIAMACHY,...	1, 3
Clouds, Aerosols	X / **D**	X	HIRDLS, MLS, OMI, TES, MODIS/MISR, SCIAMACHY, SAGE-III	1, 2, 3
Ozone (Note *B*)	X / **D**	X	HIRDLS, MLS, OMI,TES, SCIAMACHY,MIPAS,SAGE-III	1, 2, 3
CO	X	X	MLS,TES, MOPITT, MIPAS	1, 2, 3
N_2O, CO_2 CH_4, SF_6 CFCs, HCFCs	X	X	HIRDLS, MLS, TES, SCIAMACHY, MIPAS	1, 2
Short-lived organics (Note *C*)	X / **D**		TES, OMI (HCHO), SCIAMACHY	1, 2, 3
NO_x	X	X	HIRDLS, OMI, TES, SCIA	2
BrO, ClO, IO	X / **D**	X	MLS, OMI, SCIA, SAGE-III	2
HNO_3, Noy	X	X	HIRDLS, MLS, TES	2
$ClONO_2$, HCl	X	X	HIRDLS, MLS	2
SO_2			OMI,TES (volcanic)	2
^{210}Pb, ^{222}Rn, CH_3I (Note *C*)	**D** / X			1, 2, 3
Radiation (Note *D*)	X		TES,MLS,HIRDLS, ….	1, 2, 3

X indicates where existing in situ instrumentation exists.

D indicates where development is required (depending on platform choice).

* Some of the products listed in column 1 may not be obtained with sufficient precision from the space-borne instrumentation to add to TC^3 science.

Note A. Isotopic information for H_2O will provide an important constraint for understanding mixing and dehydration in the tropics.

Note B. Ozone and Aerosol curtain profiles will greatly aid in interpreting the overlap of in situ and satellite observations. A small, lightweight H_2O LIDAR would also improve the payload though this development program is expected to be significantly more difficult than an O_3/Aerosol YAG LIDAR.

Note C. Observation of numerous volatile organic compounds (VOC) and other short-lived tracers with differing photochemical lifetimes and source regions will be used to constrain the dynamics in the region of the tropical tropopause.

Note D. Broadband upward and downward radiative flux measurements with enough accuracy to determine heating/cooling rates (1 K day^{-1} or better) will help constrain heating rates. Spectrally resolved irradiance would be useful for interpretation of such a data set. Measurements of the physical properties of clouds below the aircraft will also be required for interpretation of the cooling / heating rates. This activity overlaps significantly with the goals of the proposed CRYSTAL campaign.

TC^3 observational strategy links multi-year, multi-season aircraft and balloon measurements (frequent-flyer process studies) with the global scale perspective provided by uninterrupted space-based measurements. Flight planning will be designed to integrate science and Aura validation activities by providing maximum overlap of in situ observations with satellite footprint / spatial averaging. TC^3 in situ observations will be focused on the investigation of the physical mechanisms that control the composition of the tropical upper troposphere and lower stratosphere. These studies will aid in interpreting Aura observations made at larger spatial scales. A more complete description of the TC^3 proposal can be found on the Aura website (at http://eos-aura.gsfc.nasa.gov) and at http://hyperion.gsfc.nasa.gov/Personnel/people/Kawa,_Randy/snow.html **.**

7.C.1.2 TC^3 Flight Schedule and Logistics

TC^3 will combine Aura and other satellite observations with in situ and remote aircraft observations from two Pacific deployment sites. [If the UAV Global Hawk becomes available to support this science (and payload), logistics could be streamlined.] NASA aircraft have operated out of both Hawaii and Guam and transit between these sites can be made in single flights for the ER-2. Use of the WB-57 would require a stop in Kwajalein. In any case, observations from Hawaii and Guam provide sampling of two distinct meteorological regions - areas of active convection and areas of downwelling on both sides of the ITCZ. The regions of convective activity vary seasonally. There is also strong interannual variability due to ENSO. TC^3 is envisioned as a multi-year, multi-season campaign that will provide the opportunity to sample this variability.

Observations of numerous gases (including reactive nitrogen species, H_2O and H_2O isotopes) by existing balloon payload(s) in the tropics would provide important information on the dynamics, atmospheric hydrology, and chemistry at altitudes above the aircraft ceiling. Such observations are also required for validation of Aura mid-stratospheric measurements.

TC^3 would be improved by collaboration with a tropical tropospheric campaign that could, for example, provide chemical and dynamical information at lower altitude. In situ and remote observations from the P-3 or DC-8 aircraft could be coordinated with one or more of the proposed deployments.

7.C.1.3 TC^3 Aircraft Platform

The choice of aircraft platform drives many of the logistical issues (and in some cases scientific planning) for TC^3. A number of issues remain at this time that preclude a definitive platform choice. The three possibilities:

1. ER-2. The ER-2 payload is well developed and can accomplish many of the science goals of TC^3. The payload is limited by weight, however, and adding instruments will necessitate changes in the current instrumentation or possibly the use of multiple ER-2 aircraft. The ER-2 capability near convective activity is poor and may severely limit the possibility of sampling in these conditions.

2. WB-57. The WB-57 is in many ways ideally suited to this science. The payload capability is larger (volume and weight) and it is possible to move most of the instrumentation from the ER-2 to the WB-57 (nearly transparent to the investigators) if funds for mounting the ER-2 pods on the WB-57 were made available. The future of the WB-57 program, however, remains very uncertain.

3. Global Hawk. The UAV Global Hawk would revolutionize this campaign by allowing fights to the Western Pacific and back to the U.S. without foreign deployment. It remains unclear, however, what access to this platform will be, what sampling could be done near convective systems with this platform, and how instrumentation would be developed and integrated in a timely fashion. Global Hawk remains a true wildcard for TC^3 planning.

7.C.1.4 TC^3 Schedule

We envision beginning TC^3 in summer or fall 2003 nominally coincident with the launch of Aura. This first campaign will serve to provide test opportunities for new instrumentation and to work out integration details. The experience from recent ER-2 and WB-57 campaigns suggests that integration activities can be drawn out with complex payloads. Regular and periodic campaigns would begin as early as Spring 2004 and we envision a total of 5 or 6 campaigns over a period of 2-3 years.

7.C.1.5 TC^3 Flight Planning

Independent of platform, we envision a series of flights that will combine Aura validation with science activities. We see no reason that these goals cannot be accomplished with the same flights. In Hawaii and Guam we expect to have local flights both south and north and including so-called stair-step profiles where the aircraft flies at 5 or 6 flight levels (typically dictated by Aircraft Traffic Control) over a range of about 300 km. These stacked flights would be aligned to provide maximum spatial overlap with the various satellite instruments.

7.C.1.6 TC^3 New Instrumentation

There are several constituents for which observations would improve the scientific yield from TC^3, but for which new instrumentation is needed. These are noted with 'D' in the table above. We place particular emphasis on the development of techniques for water isotope measurements, for high spatial resolution measurements (and thus high temporal resolution measurements) of short-lived organic compounds (perhaps with an improved cryogenic whole air sample). LIDAR capability for ozone, aerosol, and possibly H_2O from the high altitude aircraft is a high priority both for Aura validation, and for TC^3 science. (Although the LASE instrument is capable of providing water LIDAR measurements from the ER-2, this instrument would need to be dramatically reduced in size to accommodate the entire payload envisioned for TC^3 if a single ER-2 is to be used.) Cloud ice water measurement capability for the high altitude aircraft will be needed to evaluate the MLS product.

7.C.2 Tropospheric Missions

7.C.2.1 Two Core Missions: INTEX and LARS/TRACE-B

The emerging capability for satellite observations of the troposphere is profoundly changing the design of research aircraft missions for tropospheric chemistry. Satellite observations provide a wealth of information that can add tremendously to the value of a mission if they are properly integrated in the experimental design of the mission. At the same time, in situ measurements from the research missions offer ideal opportunities for validation of the satellite measurements, and therefore it is imperative to develop strong lines of communication between the satellite and aircraft measurement communities. The Snowmass meeting of August 1999 was designed to foster such communication in the context of Aura validation needs. This meeting spurred development of new concepts for tropospheric chemistry missions that integrate aircraft and Aura observations in a synergistic manner to address critical scientific questions, and at the same time serve Aura validation needs. Two of these mission concepts have led to detailed white papers (available from http:// www-as.harvard.edu/chemistry/trop). They are:

- INTEX: Intercontinental Chemical Transport Experiment
- LARS/TRACE-B: LBA Airborne Regional Source Experiment/Transport and Chemistry Experiment in Brazil

INTEX and LARS/TRACE-B share a common theme: to quantify the outflow of environmentally important species from major source regions to the global atmosphere. These species include greenhouse gases, oxidants, aerosols, and related gases. In the case of INTEX the region of interest is the United States; in the case of LARS/TRACE-B it is the Amazon Basin.

The objective in both missions is to relate a priori, "bottom-up" emission inventories to chemical outflow fluxes in a way that accounts for chemistry and deposition taking place within the source region. Quantitative definition of this relationship is provided by atmospheric transport and chemistry models, and the task of the missions is to test these models. The experimental design requires measurements on a hierarchy of scales (Table 7.2) and a high degree of coordination between the different measurement platforms and with the models, as illustrated in the diagram of Figure 7.5.

Table 7.2. Spatial and Temporal Scale for INTEX, LARS/TRACE-B and satellite observations.

Spatial Scale	Temporal Scale	Platform
1-10 km	Continuous (years)	Surface measurements, towers
10-1000 km	2-4 hrs daily	Small aircraft
1000-10,000 km	8-10 hrs, 2-3x/week	Large aircraft
10-10,000 km	Continuous (years)	satellites

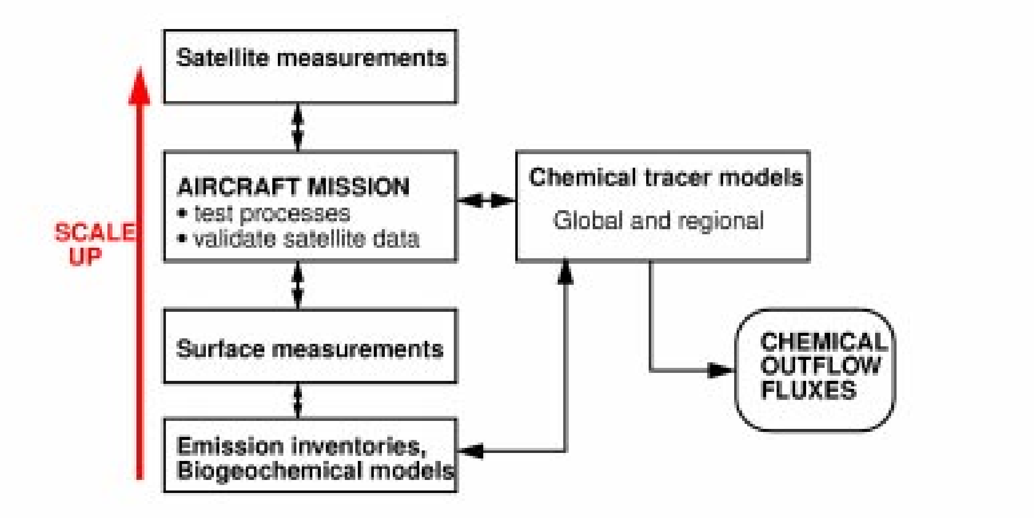


Figure 7.5. Scaling concept for INTEX and LARS/TRACE-B.

By taking advantage of the suite of measurements from ground-based, aircraft, and satellite platforms, INTEX and LARS/TRACE-B will provide the first extensive tests of our ability to scale from local processes and bottom-up inventories all the way to the global atmospheric implications. Linkage between aircraft and satellite observations will play a critical role in developing an understanding of this connectivity of scales.

The species of interest for INTEX and LARS/TRACE-B include all those for which Aura tropospheric measurements will be available, as listed in Table 7.3. Validating the Aura satellite measurements is thus a natural task for both missions. The reader is referred to the white papers of INTEX and LARS/TRACE-B for detailed presentation of the scientific objectives and proposed implementations of the missions. We give here a brief description of each mission and elaborate on the strategy for Aura validation common to both missions.

Table 7.3. Aura measurements in the troposphere.

Species	Measurement type
Ozone, CO, H_2O,T	Nadir, limb
NO, HNO_3,T	Limb (UT/LS only)
CH_4	Column (nadir)
Ozone, NO_2, HCHO, SO_2, BrO, aerosol	Column (nadir)
Ozone, H_2O, HNO_3, CH_4, aerosol, T	Limb
Ozone, H_2O, CO, HCN, T	Limb

7.C.2.1.1 INTEX: Intercontinental Chemical Transport Experiment

The northern midlatitudes continents are major global sources for a large number of anthropogenic pollutants including greenhouse gases, oxidants, and aerosols. There is a strong need to better quantify the impacts of these sources on global atmospheric chemistry and climate. A critical step is to relate our a priori knowledge of emission inventories to the actual net chemical outflow fluxes out of the source regions. Linked to this issue is the rising concern that intercontinental transport of pollution at northern midlatitudes may have significant negative implications for surface air quality in North America. To address these issues one must quantify both inflow and outflow for the region; the problem is therefore properly posed as the construction of large-scale regional budgets for the species of interest.

INTEX is part of a larger program of aircraft missions aimed at quantifying the chemical outflow from northern midlatitudes continents and the associated intercontinental transport of pollution. These missions are being coordinated under the auspices of a new IGAC activity, Intercontinental Transport and Chemical Transformation (ITCT), headed by Fred Fehsenfeld (NOAA/AL) and Stuart Penkett (U. East Anglia). INTEX will focus on North America, analyzing chemical outflow/inflow and investigating the associated continental boundary layer chemistry and ventilation processes. The scientific objectives of INTEX are as follows:

- To quantify the export and chemical evolution of radiatively and chemically important trace gases and aerosols from eastern North America to the western Atlantic, and elucidate the mechanisms and pathways associated with these transport processes;

- To quantify the impact of Asian pollution on the eastern Pacific as input to North America, and elucidate the mechanisms for these transport processes.

The first objective is central to several NASA programs including the Global Tropospheric Chemistry Program, the Aerosols and Radiation Program, and the Carbon Cycle Science program. The second objective addresses a matter of growing interest for the air pollution research community in the United States and can be expected to attract resources from NOAA, DOE, and EPA. It is intended that INTEX will draw extensively on collaboration between NASA programs and across agencies. It will also interface with parallel ITCT programs presently being developed in Europe and in eastern Asia.

The experimental design involves several aircraft operating over the United States and oceanic outflow/inflow regions, as illustrated in Figure 7.6. It involves ground-based stations in the United States to provide continuous measurements of surface air composition, and satellite measurements to place the limited aircraft measurements in a larger-scale context. The aircraft will include the NASA DC-8 for large-scale measurements of outflow and inflow, the NASA P-3 for measurements of continental boundary layer vertical fluxes and ventilation to the free troposphere, and the NASA ER-2 to examine issues of cross-tropopause transport and also to provide vertical continuity of measurement into the stratosphere for purpose of Aura validation. Additional small aircraft will provide geographical coverage for surface fluxes and boundary layer dynamics.

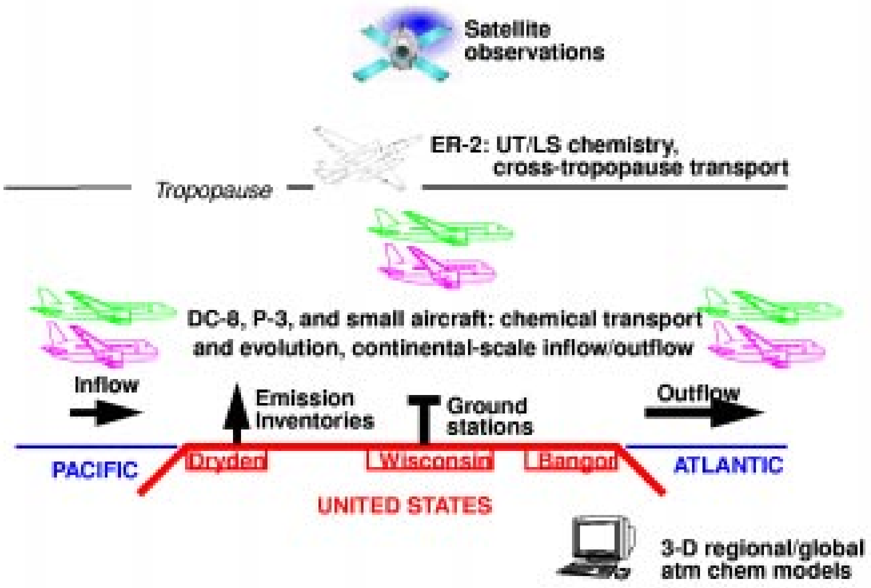


Figure 7.6. INTEX experimental concept.

The current experimental plan for INTEX involves two missions: Phase A in summer and Phase B in spring. INTEX-A mission will place particular focus on outflow from eastern North America to the North Atlantic; it should be conducted in summer when the biosphere is most active, oxidants at northern mid-latitudes are of most concern, and aerosols have the strongest radiative effects. INTEX-B will place more emphasis on long-range transport of Asian pollution across the Pacific into North America, and will be conducted in the spring when this transport is the strongest.

7.C.2.1.2 LARS/TRACE-B: LBA Airborne Regional Source Experiment/ Transport and Chemistry Experiment in Brazil

The tropical continents are of considerable importance for the global budgets of greenhouse gases, for the oxidizing power of the atmosphere, and for aerosol radiative forcing. The Amazon Basin is of particular interest in this regard because it contains the largest expanse of native moist tropical forest in the world; its mosaic of forests and wetlands represents a large source of biogenic gases to the atmosphere. It is also undergoing rapid change from deforestation and colonization. Deep convection over the region provides a fast conduit to the upper troposphere and the tropopause, which play critical roles in the Earth's climate. There is a pressing need to better quantify the sources and sinks of environmentally important species in the Amazon Basin, and the implications for the global atmosphere.

LARS/TRACE-B will address this issue within the framework of the Large-Scale Biosphere-Atmosphere Experiment in Amazonia (LBA). LBA is an ongoing US-Brazilian ground-based program focused on understanding the budgets of carbon, energy, and water vapor in the Amazon Basin. The central scientific question to be addressed by LARS/TRACE-B is as follows:

- What are the quantitative contributions of the Amazon Basin to the global atmospheric budgets of greenhouse gases, aerosols, oxidants, and their chemical precursors? This central question draws two attendant sub-questions:

- What physical, chemical, and biological processes regulate these contributions?

- What are the related implications of rapid development and exploitation of natural resources in and surrounding Amazonia?

LARS/TRACE-B cuts across the traditional Earth Science boundaries of biogeochemistry, atmospheric chemistry, atmospheric dynamics, and radiation to study a large tropical region from an integrated perspective. It will engage several programs at NASA including the Global Tropospheric Chemistry Program, the Aerosols and Radiation Program, the Biogeochemistry program. and the Carbon Cycle Science program. It will also leverage in a major way on ongoing work by Brazilian and European scientists as part of LBA. The LARS/TRACE-B mission concept was endorsed by the LBA Steering Committee in June 1999.

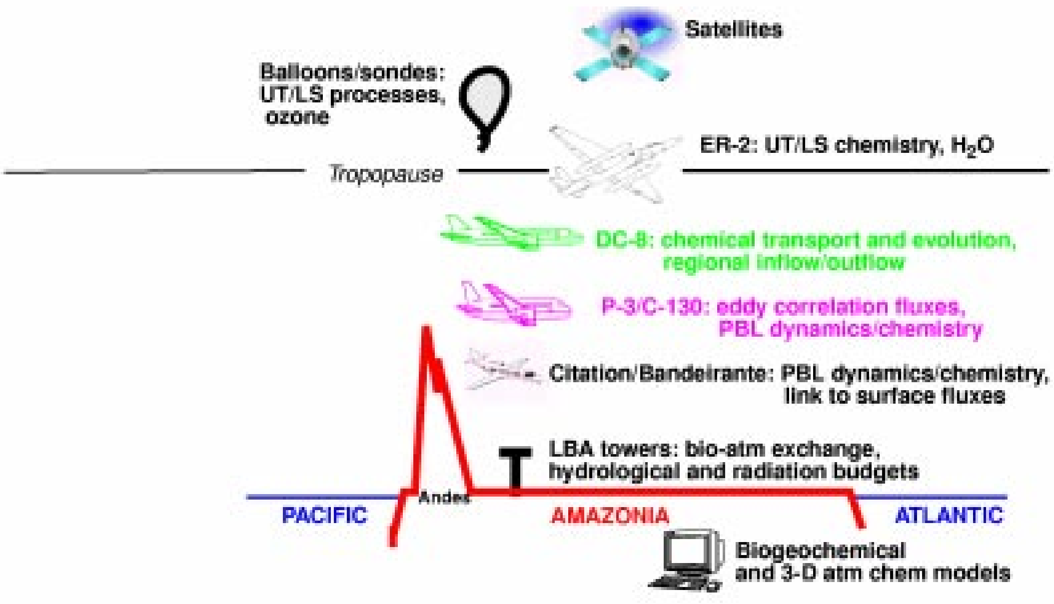


Figure 7.7. LARS/TRACE B experimental concept.

The experimental design is illustrated in Figure 7.7. Two deployments are envisioned: one at the transition from the wet to the dry season, and one at the end of the dry season (i.e., during the burning season). The mission will deploy a coordinated set of research aircraft, operating synergistically with satellite measurements and LBA ground sites, to determine regional sources and sinks of chemical species by direct measurement. The suite of aircraft will have operational capabilities from the PBL to the UT/LS. Deep convective storms occur regularly throughout the year, so that all levels of the troposphere are in direct communication with the surface and must be included in the experimental design. Four aircraft are envisioned for the mission: (1) the NASA ER-2 for the UT/LS, (2) the NASA DC-8 for the middle troposphere and continental outflow, (3) the NASA P-3 or NCAR C-130 for the lower troposphere, and (4) the UND Citation or INPE Bandeirante for the PBL.

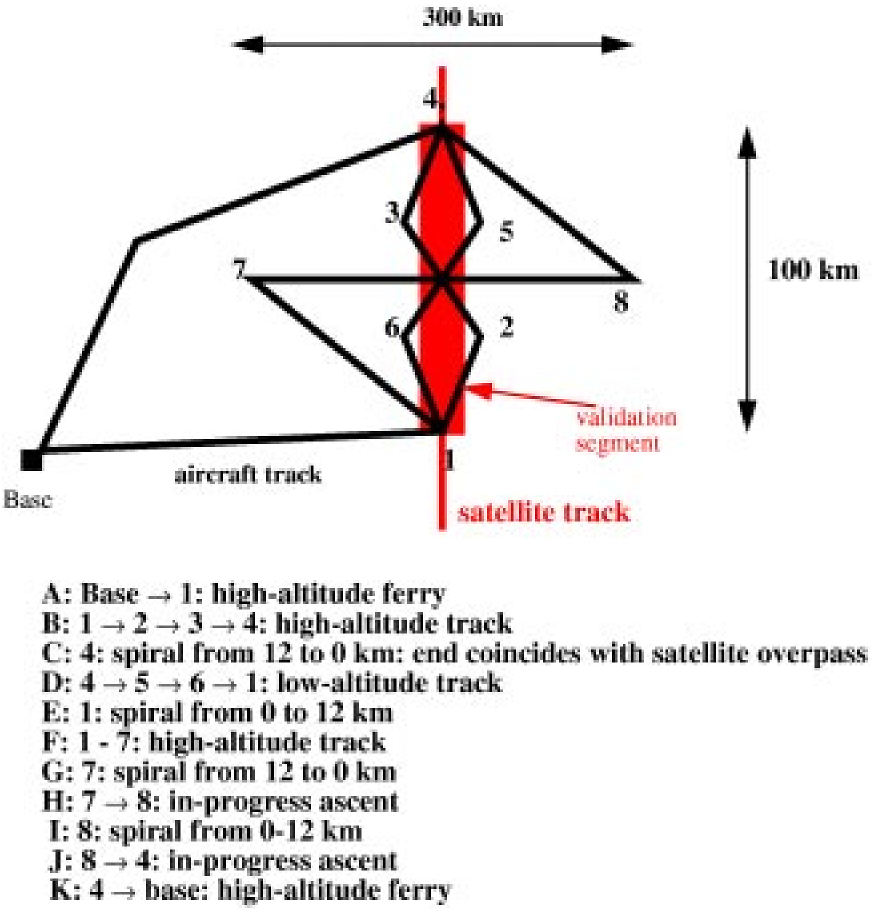
7.C.2.2 Aura Validation Strategies for INTEX and LARS/TRACE-B

Both INTEX and LARS/TRACE-B involve a close integration of in situ and satellite measurements for achieving their scientific objectives. Both involve extensive aircraft mapping of chemical composition from the surface to the lower stratosphere, over continental and oceanic environments, and with a payload including an extensive suite of gases. They are ideally suited for Aura validation, and together they can satisfy Aura validation needs for both the extratropical and tropical troposphere. The DC-8 and the ER-2 will be the key platforms for validation because of their vertical range (0-12 km and 12-20 km, respectively). Design of the validation flights must account for the unavoidable spatial and temporal mismatch between the satellite and the aircraft. A vertical profile measurement by the DC-8 flying a spiral from 0 to 12 km altitude requires about 20 minutes, but the corresponding scene is observed by the satellite in only a few seconds. Nadir views from Aura cover scenes of ~10 km horizontal extent, while limb views cover ~100 km horizontal fetches. Flying a 100 km flight track to validate the limb view at a single altitude requires 10 minutes for the DC-8.

Validation of nadir ozone and water vapor measurements can avoid the temporal mismatch problem by using airborne lidars that have been validated previously with in situ measurements. However, lidar measurement technology is not available for the other species measured by Aura (Table 7.3). Even for ozone and water vapor, the temporal mismatch problem remains for the limb measurements. Because of this problem, a requirement for successful aircraft validation of the Aura measurements is that the air composition over the satellite flight track remain stationary over the length of the in situ sampling period. An additional requirement for limb validation is that the air mass composition be horizontally homogeneous over the ~100 km limb viewing path.

An important task for the validation flight is to check that these requirements are met. Figure 7.8 presents a nominal flight pattern for Aura validation focusing on a 100-km segment of the satellite flight track. The aircraft ferries to one end of the segment (Base •1). It then flies a high-altitude zig-zag horizontal track over the segment (1 •4) during which airborne lidars check that the atmosphere is horizontally homogeneous for ozone, water vapor, and aerosols, in which case the same can be assumed for the other species. The zig-zag pattern provides a check for the assumption of horizontal homogeneity for short distances off-track. The aircraft executes a downward spiral over point 4, arriving at the surface at the time of satellite overpass. This is followed by a low-altitude zig-zag back to point 1 during which the stationarity criterion is tested using the lidar instruments, and an upward spiral at point 1 in which the stationarity criterion is tested for the species measured in situ.

The remainder of the flight track provides validation for the OMI cross-track nadir measurement. The critical component of the flight from point 1 to point 4 and back, involving two spirals, requires 1-hour flight time for the DC-8. This is the time interval over which the stationarity criterion must be satisfied. A validation experiment for Aura therefore requires an air mass devoid of clouds and with a chemical composition satisfying 1-hour stationarity and 100-km horizontal homogeneity. Over the oceans, truly cloud-free conditions are rare, and a low stratus deck is acceptable. The kind of air masses needed for Aura validation are thus subsiding air masses associated with large-scale high-pressure conditions. In these air masses the chemical composition has generally sufficient stationarity and homogeneity for our purpose, at least outside of polluted boundary layers. The meteorological conditions needed for Aura validation will frequently be found over the subtropical Pacific and Atlantic Oceans during INTEX and LARS/TRACE-B, and will also be found at least occasionally over the continental source regions.



A: Base → 1: high-altitude ferry
B: 1 → 2 → 3 → 4: high-altitude track
C: 4: spiral from 12 to 0 km: end coincides with satellite overpass
D: 4 → 5 → 6 → 1: low-altitude track
E: 1: spiral from 0 to 12 km
F: 1 - 7: high-altitude track
G: 7: spiral from 12 to 0 km
H: 7 → 8: in-progress ascent
I: 8: spiral from 0-12 km
J: 8 → 4: in-progress ascent
K: 4 → base: high-altitude ferry

Figure 7.8. Nominal flight pattern for Aura validation.

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