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"Retrieval Approach for the Tropospheric Emission Spectrometer"

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Please note: These are preliminary notes intended for internal distribution only.

Retrieval Approach for the Tropospheric Emission Spectrometer

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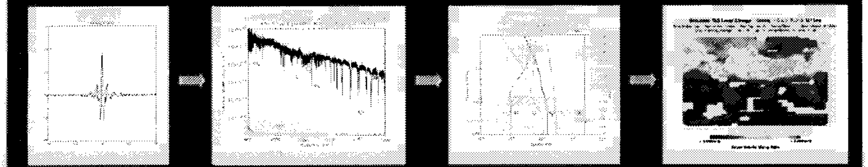
The Tropospheric Emission Spectrometer is a high-resolution Michelson interferometer designed to measure thermal emission from the atmosphere in both limb and nadir modes. It will fly on NASA's Aura satellite in 2003, together with MLS, HiRDLS and OMI. The experimental objectives are to provide a global view of the chemical state of the troposphere and UTLS regions, focussing particularly on the global distribution of tropospheric ozone and the factors that control ozone concentrations.

The spectral sampling of TES is 0.015 cm^{-1} in the limb mode, and 0.06 cm^{-1} in the nadir mode. There is an array of 16 detectors, and most of the thermal infrared is measured. The result is a very large quantity of data, about 10^6 radiances per profile, so that efficiency of data processing is paramount.

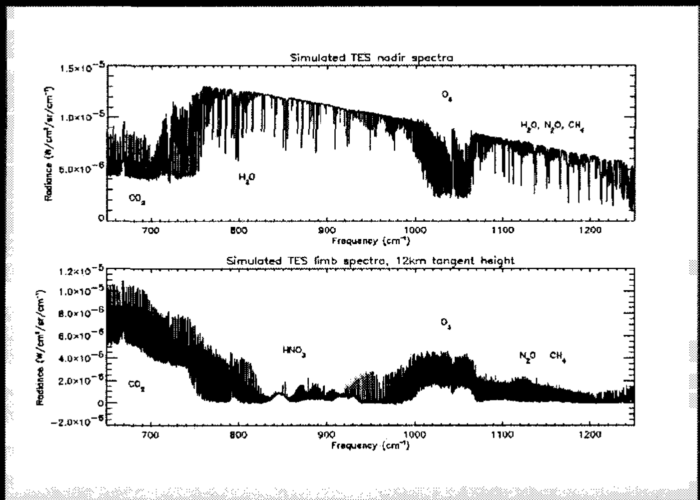
This paper will describe the methods that will be used, including the design of the forward model and its derivatives, the retrieval approach, the selection of spectral windows to be used, the error analysis.

TES Algorithm Overview

Level 1A: Produces geolocated interferograms.
Level 1B: Produces radiometrically and frequency calibrated spectra with NESR.
Level 2: Produces VMR and temperature profiles.
Level 3: Produces global maps.

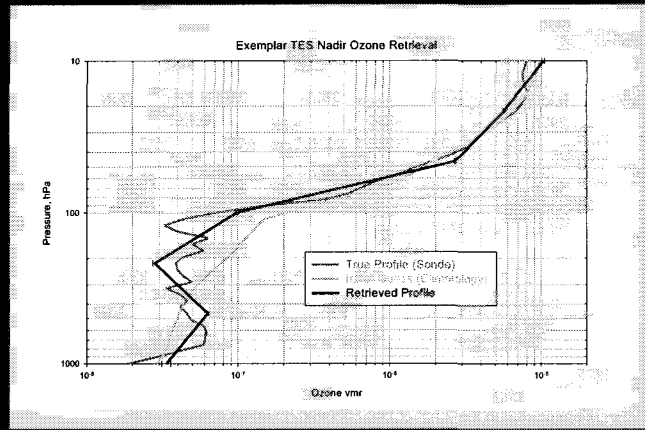


Level 1B Products



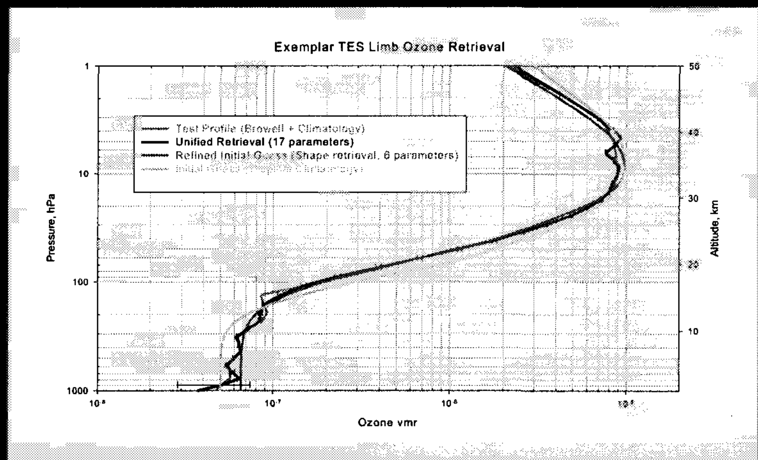
Level 2 Products

TES Nadir O3 retrievals will typically have 3 layers in the troposphere.

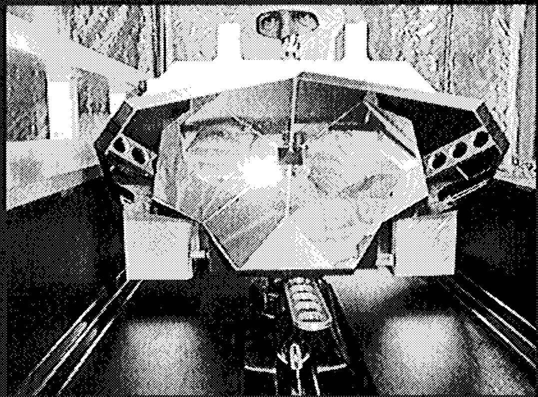


Level 2 Products

TES Limb O3 retrievals may have as many as 7 layers in the troposphere.



TES Instrument Specifications



View of the TES engineering model interferometer retroreflector

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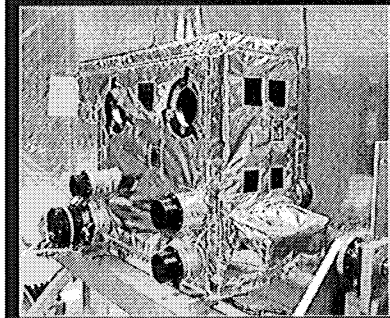
TES Interferometer and Detectors



View of the TES engineering model interferometer with thermal blanket

Spectrometer Type	Connes'-type 4-port Fourier Transform Spectrometer
Max. Optical Path Difference	± 8.45 cm (nadir & calibration) ± 33.8 cm (limb); interchangeable
Scan (integration) Time	4 sec (nadir & calibration) 16 sec (limb)
Interferogram Sampling Metrology	Nd:YAG laser
Spectral Resolution (unapodized)	0.06 cm^{-1} (nadir) 0.015 cm^{-1} (limb)
Spectral Coverage	650 to 3050 cm^{-1} (3.2 to 15.4 μm)
Detector Arrays	4 (1 x 16) arrays, optically-conjugated, all MCT PV @65K
Signal-to-Noise Ratio (spectral)	Up to 600:1 Minimum requirement is 30:1

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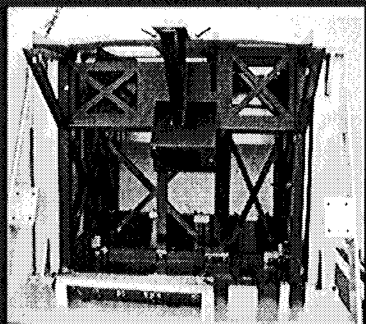
TES Allocations

Mass	385 kg
Average Power	334 W
Peak Power	361 W
Avg. Data Rate	4.5 Mbps
Peak Data Rate	6.2 Mbps
Actual Size	1.0 x 1.3 x 1.4 m (with earth shade stowed)
Lifetime	5 years on orbit



TES Structural Housing

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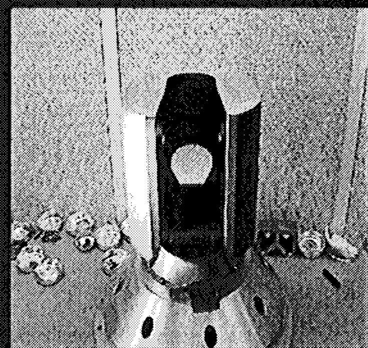
TES Pointing and Calibration

Field of Regard	45° cone about nadir; trailing limb or cold space; internal calibration sources
Pointing Accuracy	75 μrad pitch 750 μrad yaw 1100 μrad roll
Maximum Stare Time, Nadir	208 sec (40 nadir scans)
Spatial Resolution	0.5 x 5 km (nadir) 2.3 x 23 km (limb)
Radiometric Calibration	Internal, adjustable, cavity blackbody (340K) + cold space view
Radiometric Accuracy	= 1K 650 – 2500 cm^{-1} = 2K 2500 – 3050 cm^{-1}
Detector Array Co-alignment Calibration	Internal thin slit source



TES gimbal pointing mirror

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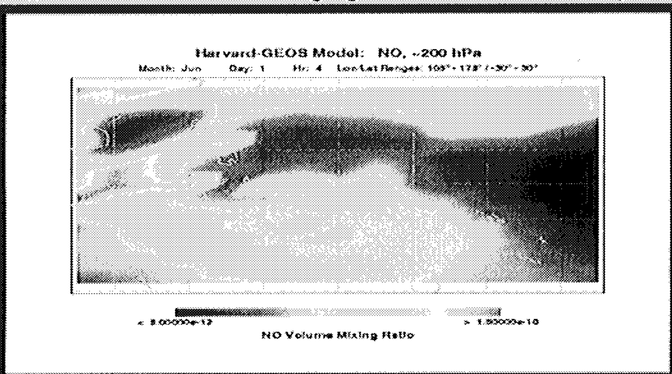
Tropospheric Chemistry Hypothesis 2: Changes in tropospheric O_3 perturb the natural abundance of OH, the main atmospheric oxidant / cleanser, with wide ranging environmental consequences.



TES will measure most of the important IR-active species in the tropospheric O_3 formation/destruction cycle, from which the OH abundance may be inferred. TES will be able to resolve different sources of O_3 precursors in the upper troposphere, e.g., biomass burning vs. non-anthropogenic sources of NOx such as lightning.

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TES Standard Products & Required Sensitivity

Product Name	Product Source: Nadir	Product Source: Limb	Required Sensitivity*
Level 1A Interferograms	✓	✓	
Level 1B Spectral Radiances	✓	✓	
Atmospheric Temperature Profile	✓	✓	0.5 K
Surface Skin Temperature	✓		0.5 K
Land Surface Emissivity†	✓		0.01
Ozone (O_3) VMR Profile	✓	✓	1 - 20 ppbv
Water Vapor (H_2O) VMR Profile	✓	✓	1 - 200 ppmv
Carbon Monoxide (CO) VMR Profile	✓	✓	3 - 6 ppbv
Methane (CH_4) VMR Profile	✓	✓	14 ppbv
Nitric Oxide (NO) VMR Profile		✓	40 - 80 pptv
Nitrogen Dioxide (NO_2) VMR Profile		✓	15 - 25 pptv
Nitric Acid (HNO_3) VMR Profile		✓	1 - 10 pptv
Nitrous Oxide (N2O) VMR profile	✓	✓	Control‡

* Sensitivity range maps to expected concentration range. NOx measurements may need averaging to meet these requirements.

† Water (and, probably, snow & ice) emissivities are known and are therefore *input*, not output parameters.

‡ Tropospheric concentration known

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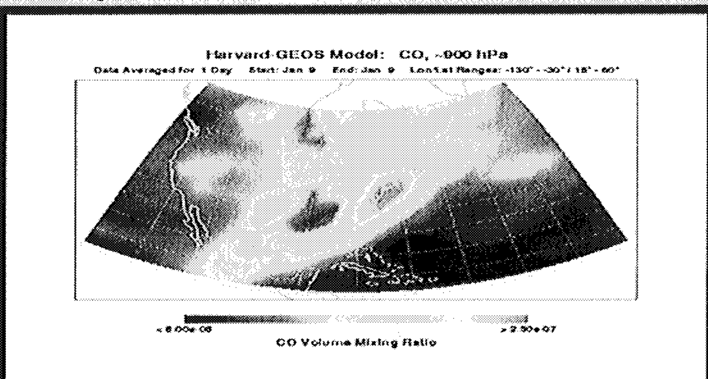
Tropospheric Chemistry Hypothesis 3: Increasing emissions of O_3 and aerosol precursors and CO will impact air quality worldwide.

- smog reduction by local emission controls could be offset by cumulative increases in global emissions.



TES will measure tropospheric carbon monoxide (CO), a major component of atmospheric pollution that will allow TES to track continental outflows.

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Potential Special (Research) Products for TES

Chemical Group	Common Name	Formula	Product Source: Nadir	Product Source: Limb
	Hydrogen Peroxide	H_2O_2		✓
H_2O_2	Monodeuterated Water Vapor	HDO	✓	✓
	Ethane	C_2H_6		✓
	Acetylene	C_2H_2		✓
	Formic Acid	HCOOH	✓	✓
	Methyl Alcohol	CH_3OH	✓	✓
	Peroxyacetyl Nitrate	$CH_3C(O)OONO_2$		✓
	Acetone	$CH_3C(O)CH_3$		✓
C-compounds	Ethylene	C_2H_4		✓
	Peroxynitric Acid	HO_2NO_2		✓
	Ammonia	NH_3	✓ *	✓
	Hydrogen Cyanide	HCN		✓
N-compounds	Dinitrogen Pentoxide	N_2O_5		✓
	Hydrogen Chloride	HCl	✓ *	
	Chlorine Nitrate	$ClONO_2$		✓
	Carbon Tetrachloride	CCl_4		✓
	CFC-11	CCl_3F	✓	✓
	CFC-12	CCl_2F_2	✓	✓
	HCFC-21	$CHCl_2F$		✓
Halogen compounds	HCFC-22	$CHClF_2$		✓
	Sulfur Dioxide	SO_2	✓	✓
	Carbonyl Sulfide	OCS	✓	✓
	Hydrogen Sulfide	H_2S	✓ *	✓
S-compounds	Sulfur Hexafluoride	SF_6		✓

* Volcanic/industrial/biomass burning plume column densities only

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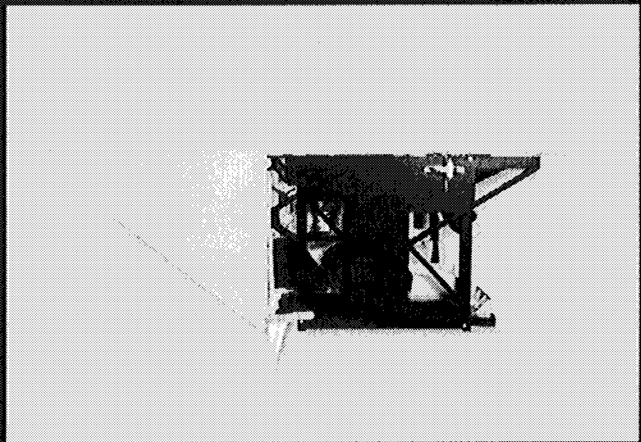
The EOS-CHEM Tropospheric Emission Spectrometer (TES)

A summary presentation of tropospheric chemistry issues and how TES measurements will contribute to their understanding



TES model in flight configuration

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Tropopheric Emission Spectrometer Formal Investigator Team

NAME	INSTITUTION	ROLE
Reinhard Beer	JPL	Principal Investigator
Shepard A. Clough	AER, Inc.	Retrieval Algorithms; Validation
Daniel J. Jacob	Harvard University	Tropospheric Chem. Modeling
Jennifer A. Logan	Harvard University	Tropospheric Chem. Modeling
Frank J. Murcray	University of Denver	Correlative Measurements; Spectroscopy
David M. Rider	JPL	Instrument Scientist; AES Team Leader
Curtis P. Rinsland	NASA Langley	Spectroscopy; Validation
Clive D. Rodgers	Oxford University	Retrieval Algorithms
Stanley P. Sander	JPL	Tropospheric Chemistry
Fredric W. Taylor	Oxford University	Strat-Trop Exchange
Helen M. Worden	JPL	Algorithm Team Leader, AES Analysis

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The TES Experiment

Global measurements of tropospheric ozone and its precursors from TES combined with *in-situ* data and model predictions will address the following key questions:

How is the increasing ozone abundance in the troposphere affecting
- *climate change?*
- *oxidizing reactions that "cleanse" the atmosphere?*
- *air quality on a global scale?*

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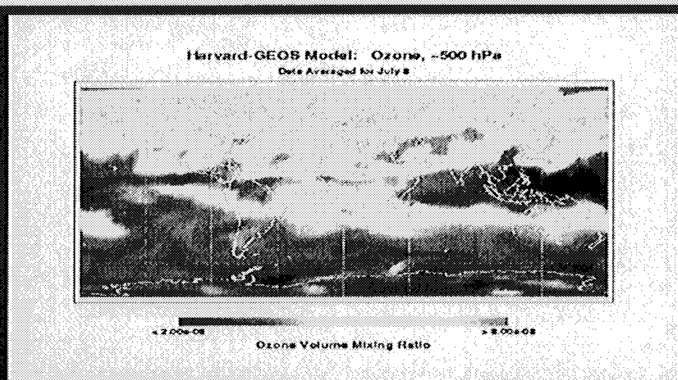
Tropospheric Chemistry Hypothesis 1: Changes in tropospheric O_3 are a significant agent for climate change.
- through direct greenhouse forcing and indirect effects on CH_4, aerosols, etc.



TES will measure vertical profiles of global tropospheric O_3 and other greenhouse gases. TES will also measure the IR radiative effects of aerosols.

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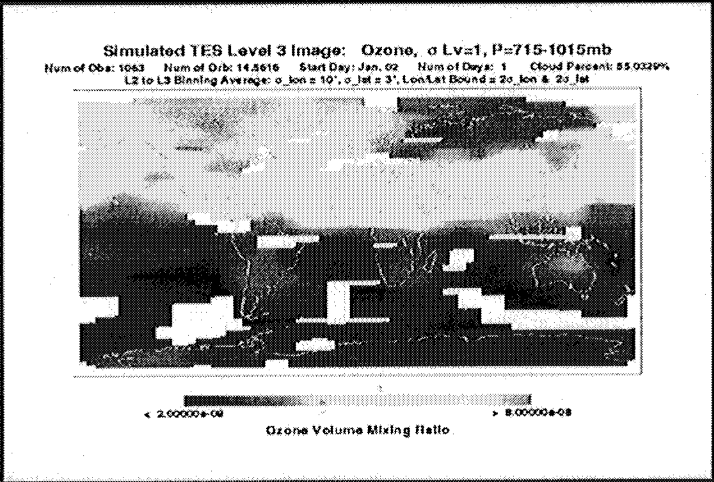
Level 3 Products



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SUMMARY

TES will provide unprecedented information about the state of the Earth's lower atmosphere.

The capability of viewing the troposphere in both limb and nadir has never before existed.

Furthermore, the spectral coverage and resolution available will permit the search for trace gases which may be indicative of unforeseen atmospheric processes.

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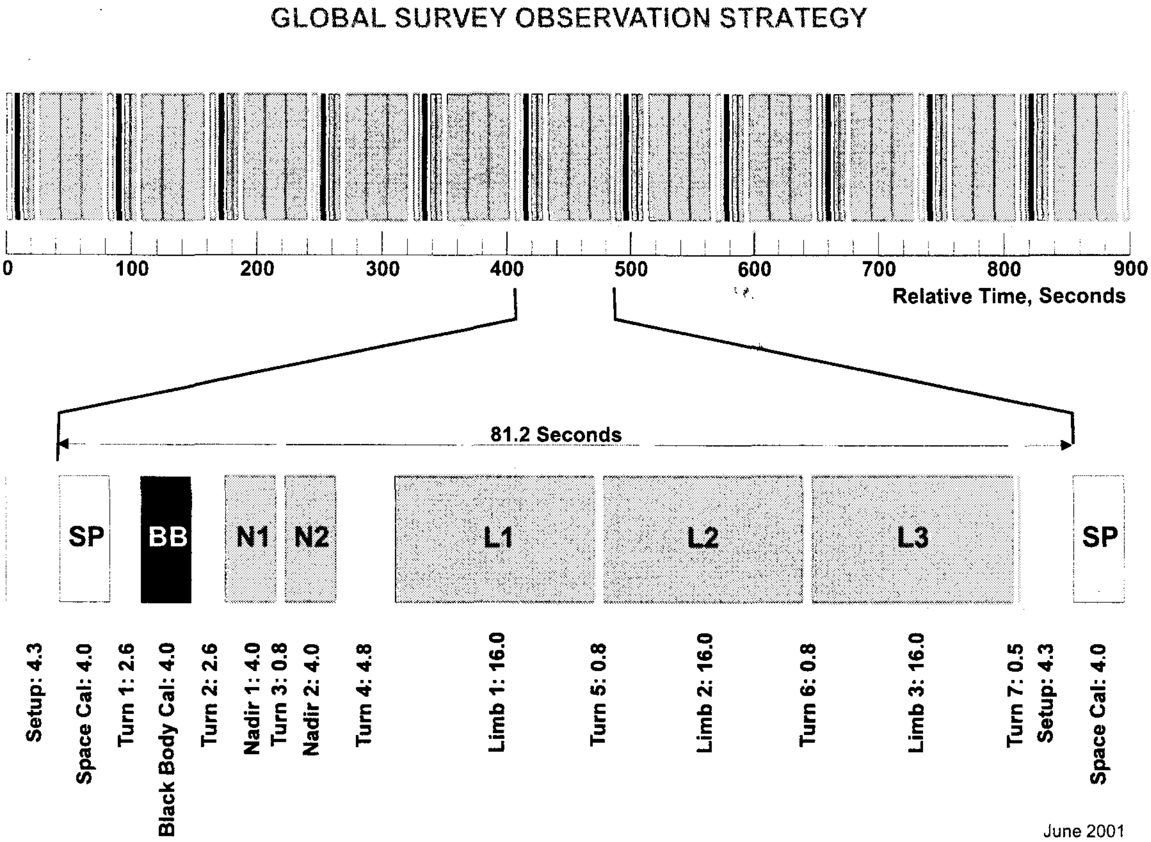
Measurement Overview

- Each orbit comprises 73 sequences of 81.2 seconds
- Each sequence contains calibration spectra, 2 nadir views and 3 limb views.
- Each view uses one of a set of filters, around 250 cm^{-1} wide, in a programmable order.
- Detectors are 16 element arrays, so each view comprises 16 spectra, either:
  - a limb array, 2.3km spacing
  - a set of contiguous nadir views, 0.5x5 km
- Spectra have resolution of 0.1 cm^{-1} (nadir) or 0.025 cm^{-1} (limb)
- Noise level around 1 K.
- Around 10^6 data points per sequence!


GLOBAL SURVEY OBSERVATION STRATEGY
0
100
200
300
400
500
600
700
800
900
Relative Time, Seconds
81.2 Seconds
SP
BB
N1
N2
L1
L2
L3
SP
Setup: 4.3
Space Cal: 4.0
Turn 1: 2.6
Black Body Cal: 4.0
Turn 2: 2.6
Nadir 1: 4.0
Turn 3: 0.8
Nadir 2: 4.0
Turn 4: 4.8
Limb 1: 16.0
Turn 5: 0.8
Limb 2: 16.0
Turn 6: 0.8
Limb 3: 16.0
Turn 7: 0.5
Setup: 4.3
Space Cal: 4.0
June 2001

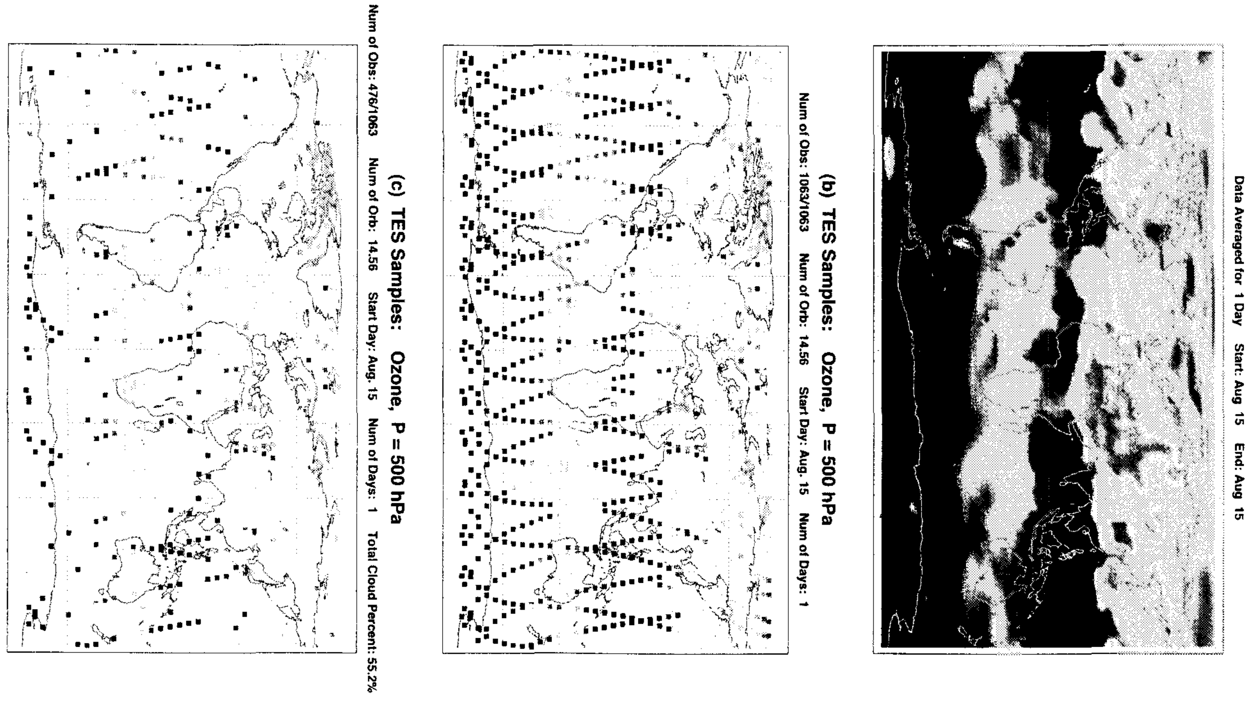

(a) GEOS-CHEM Model: Ozone, P = 500 hPa
Data Averaged for 1 Day Start: Aug 15 End: Aug 15
(b) TES Samples: Ozone, P = 500 hPa
Num of Obs: 1063/1063 Num of Orb: 14.56 Start Day: Aug. 15 Num of Days: 1
(c) TES Samples: Ozone, P = 500 hPa
Num of Obs: 476/1063 Num of Orb: 14.56 Start Day: Aug. 15 Num of Days: 1 Total Cloud Percent: 55.2%
< 2.50e-08
Ozone Volume Mixing Ratio
> 8.00e-08

Plate 1.

Building an Operational Retrieval Method

- Construct a forward model
- Determine a state vector
- Determine cost function
- Carry out characterisation & error analysis
- Select & build numerical method for minimising cost function
- Validate the resulting system

– Considering computer resources at all stages:
Time, storage,...

Forward Model

- The forward model includes:
  - Monochromatic atmospheric thermal emission model for both nadir and limb modes.
  - Instrument description
- Includes the following physics:
  - Thermal emission radiative transfer
  - Single scattering for aerosol
  - Non-LTE
  - Refraction (for limb)
  - Spectral lines of all relevant molecules
  - Continuum (water vapour)
  - Surface emission, reflectivity and elevation

  - Field of view of the instrument
  - Instrument line shape
  - Geometry of the measurement
- Evaluates Jacobians analytically, mostly

Forward Model State Vector

The forward model uses a 'full state vector,' i.e. quantities required to simulate the measured signal. Not all elements of this are retrieved.

Both views:

- Temperature on a pressure grid
- Constituent mixing ratios on a pressure grid
- Aerosol extinction coefficient on a pressure/waveno grid
- Instrument line shape
- Angular field of view function

Nadir only:

- Surface pressure
- Surface radiating temperature
- Surface optical properties: emissivity, albedo, BRDF
- Nadir view angle
- Nadir view location

Limb only:

- Spacecraft position
- Look angle of the boresight from the spacecraft
- Sun angle at nominal tangent point
- Altitude of one pressure level

Constant data:

- Constituent absorption coefficient tables on ν, p, T
- Digital elevation model
- Surface characterisation map

Radiative Transfer

- The equation of transfer is:

$$L(\Omega,\nu) = \int_0^\infty \Phi(\nu,\nu') \left\{ \int_{z_0}^\infty B(\nu',T(z)) \frac{\partial \mathcal{T}(\Omega,z,z_0,\nu')}{\partial z} dz \right.$$

(Instrument) *(Upwelling atmospheric emission term)*

$$+\left[\alpha(\nu') \int_{2\pi} \mathcal{R}_{BRDF}(\Omega,-\Omega',\nu') \int_\infty^{z_0} B(\nu',T(z)) \frac{\partial \mathcal{T}(-\Omega',z,z_0,\nu')}{\partial z} dz\, d\Omega'\right.$$

(Downwelling, back – reflected, atmospheric emission term)

$$+\varepsilon(\Omega,\nu') \cdot B(\nu',T_{surf})$$

(Surface emission term)

$$\left.\left. +\alpha(\nu') \cdot \mathcal{R}_{BRDF}(\Omega,-\Omega_0,\nu') \cdot E_s(\nu') \cdot \Omega_s \cdot \mathcal{T}(-\Omega_0,\infty,z_0,\nu')\right] \mathcal{T}(\Omega,z_0,\infty,\nu') \right\} d\nu' \tag{3.5}$$

(Reflected sunlight term)

where

- $L(\Omega,\nu)$ = radiance at frequency ν into upward, directed, solid angle Ω
- $\Phi(\nu,\nu')$ = ILS, i.e. spectral response of ν due to incident radiance at ν'
- $B(\nu,T)$ = Planck function for temperature T
- T_{surf} = surface temperature
- $\mathcal{T}(\Omega,z,z',\nu')$ = atmospheric transmittance at frequency ν' in a direction Ω between altitudes z and z'
- $\alpha(\nu')$ = surface albedo
- $\mathcal{R}_{BRDF}(\Omega,-\Omega',\nu')$ = surface biconical reflectance function for incident (downward) solid angle $-\Omega'$ and emergent (upward) solid angle Ω
- $\varepsilon(\Omega,\nu')$ = surface emittance at frequency ν' in the upward direction Ω
- $E_s(\nu')$ = disk-average solar radiance
- Ω_s = solar solid angle at Earth

The same equation holds for limb emission sounding if the last three (surface-related) terms are omitted. While the equation, therefore, seems much simpler, the geometry of the light path (especially in the lower atmosphere) becomes much more complicated because of strong refraction effects.

but I won't go over this in detail...

Radiative Transfer 2

- This must be evaluated monochromatically and then integrated over angle and wavenumber:

$$L = L_0 \exp(-\tau_0) + \int B(\tau)\exp(-\tau)d\tau$$

- Numerically this is evaluated in a way which is based on the differential form of the equation of transfer, $dL/d\tau = B-L$:

$$L_{i+1} = L_i T_i + B_i^e(1 - T_i)$$

where:

T_i is the transmittance of the ith layer, i.e. $\exp(-\tau_i)$

τ_i is the optical depth of the ith layer,

B^e is the effective Planck function of the layer (an approximation to $B(\tau)$ weighted with $\exp(-\tau)$ across the layer)

- For speed, both $B(\nu,T)$ and exp are pretabulated rather than being

Optical Depth Calculation

- Optical depth is $\tau = \int k(\nu,p,T)du$, where u is absorber amount.

- The calculation of the absorption cross-section $k(\nu,p,T)$ can be time or storage consuming. Options are:

  – Calculate it line-by-line

    Takes a lot of time - HITRAN has a lot of lines!

  – Precompute it, and store it as cross-section tables

    Takes a lot of space:

    Point spacing ~ 10^{-4} cm^{-1}, 2000 cm^{-1} gives 2×10^7 points
    50 pressures, 10 temperatures, 40 gases gives 4×10^{11}...

- TES has chosen to store cross-section tables for microwindows in the operational code.

Path Integrals and Ray Tracing

Path Integrals

The optical depth calculation requires an integral along the path of the ray from/to the satellite:

$$\int k(\nu,p,T)\,(\mathrm{d}u/\mathrm{d}x)\,\mathrm{d}x$$

This requires knowledge of the ray, as well as an efficient method of doing the integrals.

Ray Tracing

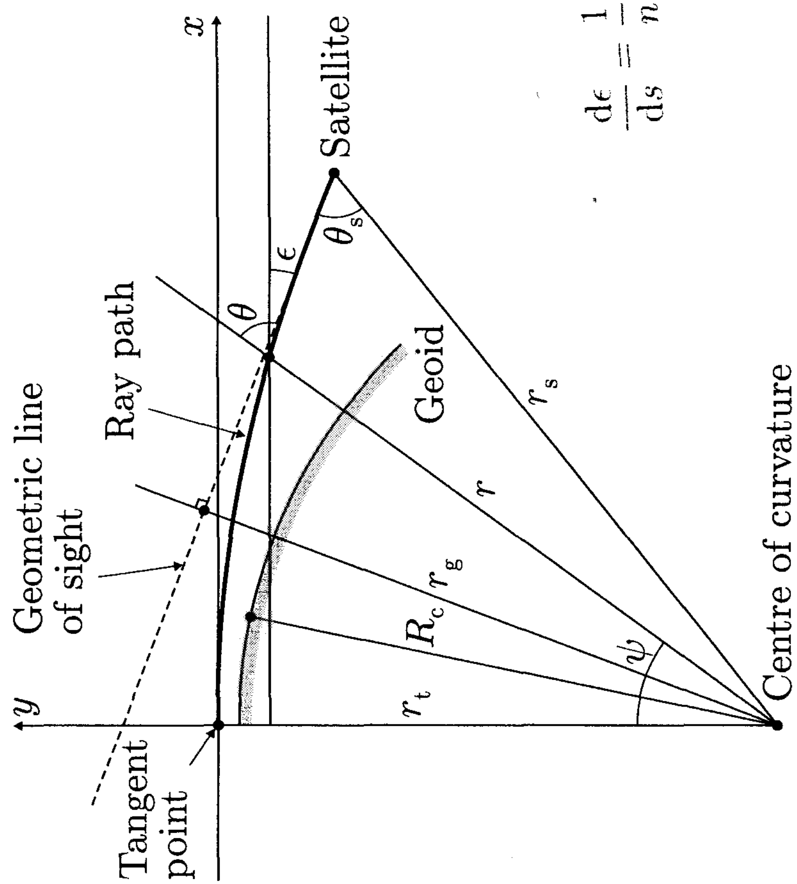
Nadir view: Straightforward spherical trigonometry.
Refraction is negligible.

Limb view: Refraction is important.

Jacobians

– It is possible, but complicated, to evaluate analytic derivatives of the ray trace and the path integrals

– This is such a small part of the forward model that the perturbation methods is not computationally expensive.



$$\frac{\mathrm{d}\epsilon}{\mathrm{d}s} = \frac{1}{n}\left(\frac{\partial n}{\partial t}\right)_s$$

Field of View Integration

- Nadir: This is unimportant, because the state vector doesn't vary within the instrument field of view.
- Limb: The atmospheric limb radiance profile varies significantly over the field of view, so the integration has to be carried out.
- For the horizontally homogeneous case
  - consider rays from each tangent point pressure level to the satellite
  - refraction equation provides an angle θ_s of the ray at the satellite

$$\sin \theta_s = n(r_t) r_t / r_s$$

where tangent point has refractive index n at radius and the satellite is at r_s

  - ray trace from each tangent point pressure level (hydrostatic eqn first!) to satellite altitude, and compute radiance spectrum
  - integrate over angle on an unequally spaced grid using a four point Lagrange interpolation for the radiance to the grid that the FOV is stored on.
- The horizontally inhomogeneous case is seriously messy.

Retrieval Method Outline

- The usual nonlinear least squares to minimise the cost function:

$$J = (\mathbf{y} - \mathbf{F}(\mathbf{x},\mathbf{b}))^T \mathbf{S}_e^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x},\mathbf{b})) + (\mathbf{x} - \mathbf{x}_0)\mathbf{H}(\mathbf{x} - \mathbf{x}_0)$$

  - with respect to $\mathbf{x}$
  - $\mathbf{y}$ is a subset of the spectral data
  - $\mathbf{S}_e$ is the measurement noise: diagonal
  - $\mathbf{H}$ and $\mathbf{x}_0$ may be *ad hoc* constraints or statistical *a priori*
- Minimisation uses Levenberg-Marquardt method
- An *ad hoc* 'shape retrieval' using a simplified state vector provides a first guess.
- The subset of the spectrum used comprises 'microwindows' – limited regions in wavenumber and tangent altitude (limb case) containing

Retrieval Strategy

• Retrieval process is table-driven

• Each stage of retrieval is defined by such things as:

– Shape retrieval or full retrieval

– Subset of products to be jointly retrieved
(e.g. T, ozone, etc)
– Constraints
(e.g. Tikhonov, climatology, forecast,...)
– Microwindows

– First guess
(e.g. climatology, forecast, previous stage, previous retrieval...)

– Products to be stored or archived

• A typical table might provide for retrieval stages as follows:
1. Pointing and temperature around the tropopause (limb)
2. Pointing and temperature (limb)
3. Temperature and water (nadir)
4. N2O limb & column (cloud check)
5. Ozone (limb)
6. Other constituents in some order TBD
n. Ozone (nadir)

Retrieved State Vector

The retrieval state vector is a subset of the full state vector:

Both views:
– Temperature on a subset pressure grid
– Constituent log mixing ratios on a subset pressure grid
– Aerosol extinction coefficient on a subset pressure/waveno grid

Nadir only:
– Surface emitting temperature per detector
– Surface emissivity

Limb only:
– Look angle of the boresight from the spacecraft

Temperature and log mixing ratio are linear in ln(p)

Quantities not retrieved are treated as forward model parameters for the purpose of error analysis.

Capturing Tropospheric Ozone TimeVariability

A Study Using TES Nadir Retrievals.

K. Bowman[1], J. Worden[2], T. Steck[1], H. Worden[1], S. Clough[2], C. Rodgers[3]
[1]Jet Propulsion Laboratory, Pasadena, CA.
[2]Atmospheric and Environmental Research, Cambridge, MA.
[3]Oxford University, Oxford, England.

Goal and assumptions of study

- Determine, with simulated retrievals, whether retrieved TES nadir retrievals are sensitive enough to capture the time variability in a set of "real" ozone measurements.
- Assumptions for study:
  - Surface temperature, atmospheric temperature, and water amounts have been accurately retrieved prior to the ozone retrievals. Temperature errors, however, are quantified for ozone retrievals.
  - The signal-to-noise (SNR) ratio is 300, which is based on a conservative radiometric model
  - There are no spectral systematic biases.

Retrieval problem

- Given: $\mathbf{y} = \mathbf{F}(\mathbf{x}) + \mathbf{n}$ where **y** is the measured spectrum, **x** is the true ozone profile, **F** is the forward model, and **n** is additive white Gaussian noise. The retrieval problem is to find **x** given **y**.
- The fine vertical structure and variability of ozone profiles lead to nonlinearities in the retrieval that result in numerical instabilities or unacceptably expensive computations. We address these problems by separating the retrieval into two steps.

2-step retrieval

- First, estimate the broad features of the ozone using the "shape retrieval"

$$\hat{\mathbf{x}}_s = \mathbf{M}_s \cdot \min_z \left\| \mathbf{y} - \mathbf{F}(\mathbf{M}_s \mathbf{z}_s) \right\|^2_{\mathbf{S}_\epsilon^{-1}}$$

- Second, estimate the fine features using a "level" retrieval with smoothing constraint.

$$\hat{\mathbf{x}} = \mathbf{M}_z \cdot \min_z \left(\left\| \mathbf{y} - \mathbf{F}(\mathbf{M}_z \mathbf{z}) \right\|^2_{\mathbf{S}_\epsilon^{-1}} + \left\| \mathbf{z} - \mathbf{M}_z^* \hat{\mathbf{x}}_s \right\|^2_{\Lambda} \right)$$

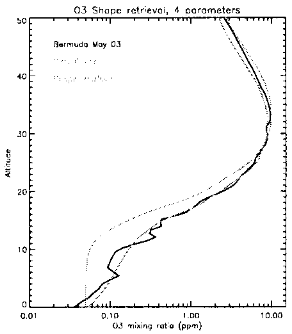
2-step retrieval (con't)

- The retrieval minimizes the cost function with respect to the retrieval vector $\mathbf{z}_s$ for the shape retrieval, and $\mathbf{z}$ for the level retrieval.
- The retrieval vectors are mapped to the ozone profile, $\mathbf{x}$, through $\mathbf{M}_s$ for the shape retrieval and $\mathbf{M}_z$ for the level retrieval.
- The level retrieval uses a smoothness constraint based on the Tikhonov-type constraint matrix Λ and constraint vector $\mathbf{M}_z^* \hat{\mathbf{x}}$

Shape Retrieval

- We retrieve four parameters:

1. A scaling parameter that scales a pre-configured stratospheric profile
2. A "shift" parameter that vertically adjusts the pre-configured stratospheric profile.
3. A scaling parameter for the troposphere
4. Tropospheric lapse rate.



Regularization of level retrieval

- A Tikhonov-type constraint is used to insure a smooth estimate.
- Constraint scaled by the atmospheric profile for smoothness in the troposphere
- Strength calculated based on estimated error.

$$\Lambda = \alpha \mathbf{B}^{-1}\mathbf{L}^T\mathbf{L}\mathbf{B}^{-1}$$

$$\mathbf{L}^T\mathbf{L} = \begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & 0 & -1 & 2 \end{pmatrix}$$

$$[\mathbf{B}]_{ii} = \left[\mathbf{M}_l^* \hat{\mathbf{x}}_s\right]_i$$

Error analysis

- Estimate from shape retrieval is used as initial guess and *a priori* to level retrieval.
- Hence, error analysis must be extended to handle a variable *a priori*.

Linear retrieval

The linear estimate of the 2-step retrieval is

$$1.\ \mathbf{x}_s = \mathbf{x}_0 + \mathbf{A}^s_{xx}(\mathbf{x}^* - \mathbf{x}_0) + \mathbf{M}_s\mathbf{G}_s\mathbf{n}$$

$$2.\ \hat{\mathbf{x}} = \mathbf{x}_s + \mathbf{A}^z_{xx}(\mathbf{x}^* - \mathbf{x}_s) + \mathbf{M}_z\mathbf{G}_z\mathbf{n}$$

where $\mathbf{A}^z_{xx}$ and $\mathbf{A}^s_{xx}$ are the averaging kernels, $\mathbf{G}_z$ and $\mathbf{G}_s$ are the gain matrices, $\mathbf{M}_z$ and $\mathbf{M}_s$ are the maps for the level and shape retrieval, respectively. $\mathbf{x}_0$ is the initial guess, $\mathbf{x}^*$ is the true profile, $\mathbf{x}_s$ is the estimate from the shape retrieval, and $\hat{\mathbf{x}}$ is the estimate of the ozone.

Error for 2-step retrieval

The error in the linear estimate is

$$\tilde{\mathbf{x}} = \hat{\mathbf{x}} - \mathbf{x}^* = \underbrace{(\mathbf{A}^z_{xx} - \mathbf{I})}_{\text{Smoothing error}}(\mathbf{x}^* - \mathbf{x}_s) + \underbrace{\mathbf{M}_z\mathbf{G}_z}_{\text{Noise error}}\,\varepsilon.$$

The total error covariance is then

$$\mathbf{S}_{\tilde{x}} = \underbrace{(\mathbf{I}-\mathbf{A}^z_{xx})(\mathbf{I}-\mathbf{A}^s_{xx})\mathbf{S}_{x^*}(\mathbf{I}-\mathbf{A}^s_{xx})^T(\mathbf{I}-\mathbf{A}^z_{xx})^T}_{\text{Smoothing error}}$$

$$\underbrace{+\left[\mathbf{M}_z\mathbf{G}_z - (\mathbf{I}-\mathbf{A}^z_{xx})\mathbf{M}_s\mathbf{G}_s\right]\mathbf{S}_e\left[\mathbf{M}_z\mathbf{G}_z - (\mathbf{I}-\mathbf{A}^z_{xx})\mathbf{M}_s\mathbf{G}_s\right]^T}_{\text{Noise error}}.$$

Column error

- The column amount is simply $\hat{\mathbf{c}} = \mathbf{H}\hat{\mathbf{x}}$. The error $\tilde{\mathbf{c}} = \hat{\mathbf{c}} - \mathbf{c}$ is then

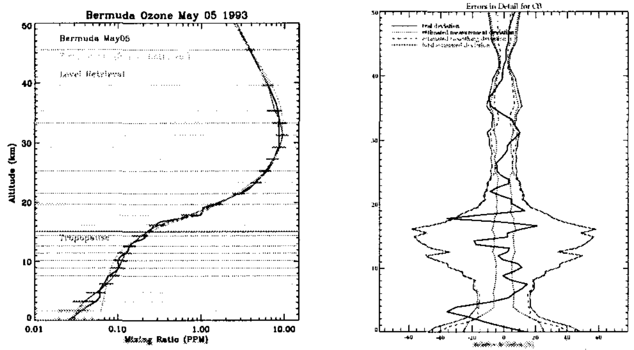
$$\mathbf{S}_{\tilde{c}} = \mathbf{H}\mathbf{S}_{\tilde{x}}\mathbf{H}^T$$

- The column operator, **H**, can be calculated for any region of the atmosphere.

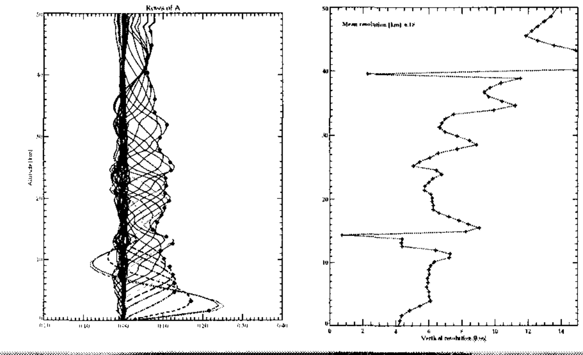
Simulation of Radiances

- Radiances calculated from ozone-sondes released over Bermuda from April 14, 1993 to May 25, 1993 [1,2]. These sondes included profiles of temperature, water, and ozone.
- Profiles mapped to UARS pressure grid:
  $\log p = 3 - i/N,\quad N=24,\ i=0,\ldots,85.$
- URAP climatology added to ozone-sonde data from 10 mb to .1 mb [3].

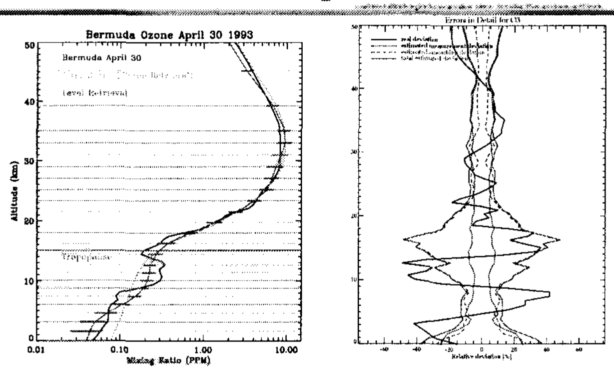
Retrieval May 05, 1993



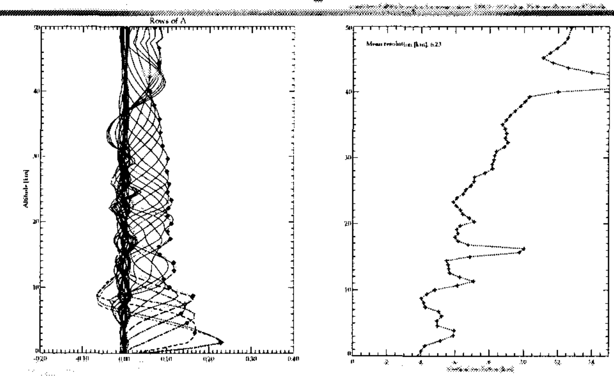
Resolution of May 05 retrieval



Retrieval April 30, 1993



Resolution of April 30 Retrieval



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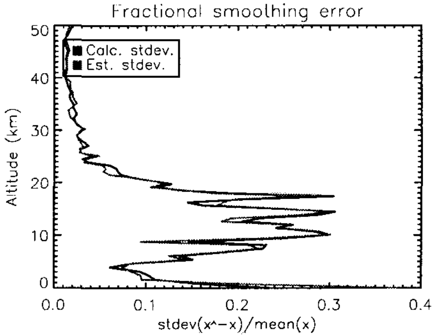
Smoothing error



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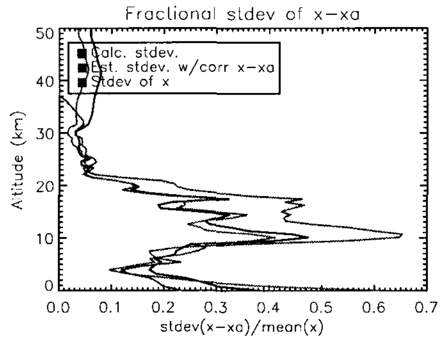
Error in x-xs



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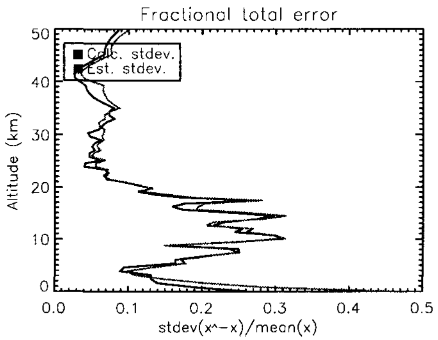
Total Ensemble error



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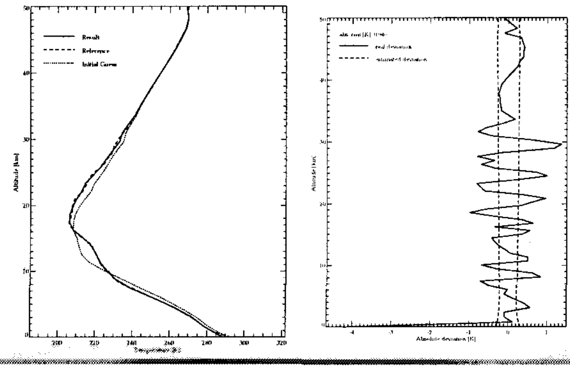
Temperature retrieval-April 30



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Error in ozone retrieval

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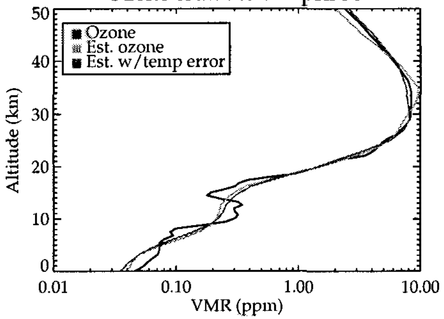
Ozone estimate of April 30.



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Column retrievals of troposphere

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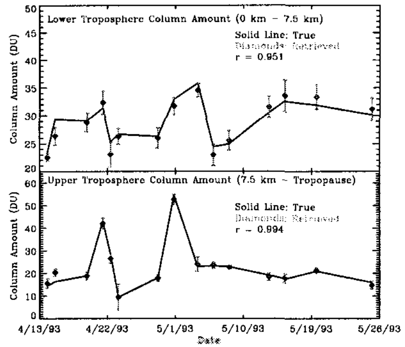

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Conclusions

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- 15 ozone-profiles were estimated using nadir simulated radiances.
- We employed a novel 2-step retrieval algorithm that is robust to significant deviations between initial guess and the true ozone profile.
- The average resolution was about 6 km leading to about 2 pieces of information in the troposphere.
- The retrieved columns in the lower and upper troposphere were correlated at .95 and .99, respectively.

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References

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[1] Dataset obtained from private communication with Jennifer Logan, Harvard University.

[2] S.J. Oltmans, *et al.,* "Summer and spring ozone profiles over the North Atlantic from ozonesonde measurements", J. Geophys. Res., 101: (D22) 29179-29200 Dec 20 1996

[3] http://hyperion.gsfc.nasa.gov/Analysis/UARS/urap/home.html

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