

Capturing Tropospheric Ozone Time Variability: A Study Using TES Nadir Retrievals

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Abstract: We perform nadir retrievals of ozone using simulated radiances from ozone-sondes over Bermuda from April 14 to May 25, 1993. Using a novel two-step retrieval strategy, we characterize the sensitivity of TES nadir retrievals to time variations of ozone.

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OCIS codes: (1280.0280) Remote sensing, (999.9999) atmospheric ozone retrievals

1. Introduction

The Tropospheric Emission Spectrometer (TES) on the EOS-Aura spacecraft is an infrared Fourier Transform Spectrometer (FTS) that will record the Earth's spectral radiance from discrete locations along the orbit track in the frequency range 650 to 2250 cm^{-1} , (15.4 to 4.4 μm) [1]. The goal of this study is to determine, with simulated spectra, whether retrieved TES nadir ozone profiles are sensitive enough to capture the time variability observed in a set of real ozone measurements. To that end, we have acquired a set of 15 ozone sonde profiles from the Bermuda station taken between April 14 and May 25, 1993[2]. Each ozone-sonde profile set of temperature, H_2O , and ozone are mapped to the UARS pressure levels: $\log p_i = 3 - i/N$, where $N=24$ and $i = 0, \dots, 23$. This mapping keeps the integrated ozone column amounts between pressure levels consistent with the column amounts of the original ozone-sonde altitude grid. Because the ozone-sonde profiles only take measurements up to 10 millibars and the UARS pressure grid extends to 0.1 millibars, it is necessary to incorporate a realistic ozone profile between 10 and 0.1 millibars. Therefore, a URAP ozone climatology profile [3] is scaled onto the corresponding low pressure levels. Since TES will have a near repeat view of its nadir targets--separated by about 1° longitude--every 2 days, this set of ozone-sonde data, which is taken approximately every other day, provides a reasonable simulation of TES temporal sampling.

Assumptions about the instrument and model are required for any simulation. For this simulation we assume that (1) surface temperature, atmospheric temperature, and water amount have been accurately retrieved prior to the ozone retrievals. However, systematic errors from the retrieval of temperature are included in the error analysis as forward model parameter errors [4]. (2) The signal-to-noise ratio (SNR) is 300; this SNR is much less than the optimal TES SNR of 1000, obtained by averaging radiances from all 32 pixels. The reduction accounts for the estimated precision of the radiative transfer calculation. Gaussian white noise, with a standard deviation of $1.32 \times 10^{-8} \text{ W (cm}^2 \text{ sr}^{-1} \text{ cm}^{-1})$, is added into the simulated radiances associated with each ozone-sonde profile to account for this specific SNR. (3) There are no systematic errors associated with the instrument calibration or molecular line parameters. This last assumption might be unrealistic, but is necessary until multiple cross-comparisons with other satellite, ground-based, and aircraft measurements, permit the accurate characterization of these errors.

2. Two-step retrieval strategy

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.

This first step estimates the broad features of the ozone using a technique that we call the “shape retrieval”. The ozone profile shape is unique in that the mixing ratio and number density peaks in the stratosphere (about 33 km). We take advantage of this prior knowledge of ozone formation by constructing a set of retrieval parameters that are specific to the stratosphere and troposphere and that retrieve aspects of the ozone profile shape. In the stratosphere, we retrieve two parameters: (1) a scaling parameter that scales a pre-configured stratospheric profile and (2) a “shift” parameter that vertically adjusts the pre-configured stratospheric profile. We also retrieve two parameters associated with the troposphere: a scaling parameter and the ozone lapse rate. In this context we treat the stratosphere and troposphere as two separate atmospheres. We also calculate the sensitivities of these parameters with respect to the forward model.

The second step consists of retrieving a linear piece-wise approximation to the ozone profile that is constrained by a Tikhonov-type regularization[5] and by a constraint vector that is set to the ozone estimate of the shape retrieval. These steps are summarized as

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

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

where $\mathbf{F} : \mathbb{R}^M \rightarrow \mathbb{R}^N$ is the forward model, $\mathbf{z}_s \in \mathbb{R}^M$ is the shape retrieval vector, $\mathbf{M}_s \in \mathbb{R}^{M \times M}$ is the shape retrieval mapping matrix, $\mathbf{y} \in \mathbb{R}^N$ is the measured spectral radiance vector, $\mathbf{S}_e \in \mathbb{R}^{N \times N}$ is the measurement error covariance matrix, Λ is the Tikhonov constraint matrix, $\mathbf{M}_l \in \mathbb{R}^{M \times M^*}$ is a piece-wise linear mapping matrix, $\mathbf{M}_l^* \in \mathbb{R}^{M^* \times M}$ is its pseudo-inverse, \mathbf{z} is the retrieval vector for the piece-wise linear retrieval, and $\hat{\mathbf{x}}$ is the estimate of the ozone profile on the full-state vector—a finely spaced vertical log pressure grid on which the forward model is evaluated.

The error covariance of the two-step retrieval, which takes into account the time-varying constraint vector, is

$$\begin{aligned} \mathbf{S}_{\hat{\mathbf{x}}} = & \left[(\mathbf{I} - \mathbf{A}_{xx}) \mathbf{A}_{xx}^s + \mathbf{A}_{xx} \right] \mathbf{S}_x \left[(\mathbf{I} - \mathbf{A}_{xx}) \mathbf{A}_{xx}^s + \mathbf{A}_{xx} \right]^T \\ & + \left[(\mathbf{I} - \mathbf{A}_{xx}) \mathbf{M}_s \mathbf{G}_s + \mathbf{M} \mathbf{G}_z \right] \mathbf{S}_e \left[(\mathbf{I} - \mathbf{A}_{xx}) \mathbf{M}_s \mathbf{G}_s + \mathbf{M} \mathbf{G}_z \right]^T, \end{aligned} \quad (3)$$

where $\mathbf{A}_{xx} = \partial \hat{\mathbf{x}} / \partial \mathbf{x}$, $\mathbf{A}_{xx}^s = \partial \hat{\mathbf{x}}_s / \partial \mathbf{x}$, $\mathbf{G} = \partial \mathbf{z} / \partial \mathbf{y}$, $\mathbf{G}_s = \partial \mathbf{z}_s / \partial \mathbf{y}$ are the averaging kernels and gain matrices of the level retrieval and shape retrieval respectively [4]. The column is related to the ozone estimate in equation (2) through the column operator, \mathbf{H} such that $\hat{\mathbf{c}} = \mathbf{H} \hat{\mathbf{x}}$. The error for column is then simply

$$\mathbf{S}_{\hat{\mathbf{c}}} = \mathbf{H} \mathbf{S}_{\hat{\mathbf{x}}} \mathbf{H}^T. \quad (4)$$

3. Results

Fig. 1 shows the results of the retrieval of ozone on April 30th, 1993, which contains interesting structure in the troposphere. The initial guess for the two-step retrieval is a combination of the AFGL standard ozone profile in the stratosphere and a constant .05 ppm profile in the troposphere. The estimate from the shape retrieval is then used as both an initial guess and constraint vector for the piece-wise linear retrieval. The resolution of the retrieval was calculated from the averaging kernel to be approximately 6 km.

This resolution provides roughly 2 pieces of information in the troposphere. This information is represented as columns in Fig. 2 where the error bars were calculated using equation (4). The retrieved columns capture the time-variability of the true columns; the correlation is 0.99 in the upper troposphere and .95 in the lower troposphere.

4. References

- [1] R. Beer, T.A. Glavich and D.M. Rider, “Tropospheric Emission Spectrometer (TES) for the Earth Observing System (EOS) Aura Satellite. I. Objectives, Requirements and Instrument Overview”, submitted to Applied Optics, March 2000.
- [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.esfc.nasa.gov/Analysis/UARS/urap/home.html>
- [4] C. D. Rodgers, *Inverse Methods for Atmospheric Sounding: Theory and Practice*, (World Scientific, London, 2000)
- [5] T. Steck and T. von Clarmann, Regularisation of MIPAS-ENVISAT offline constituent retrieval: Strategy and diagnostics. To be published in the proceedings of the International Radiation Symposium (IRS 2000).

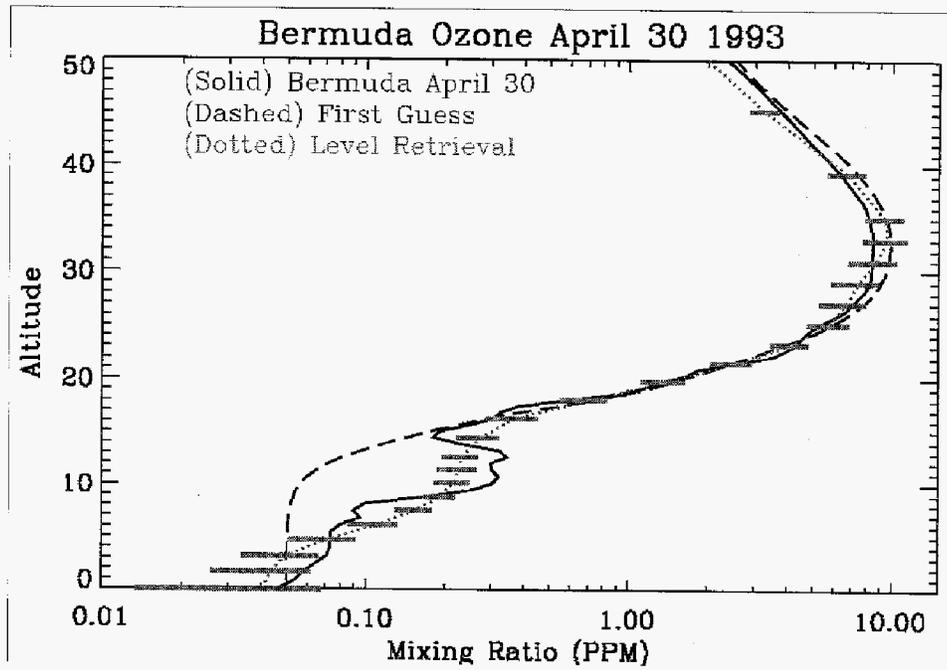


Fig 1. Retrieval of ozone over Bermuda on April 30, 1993.

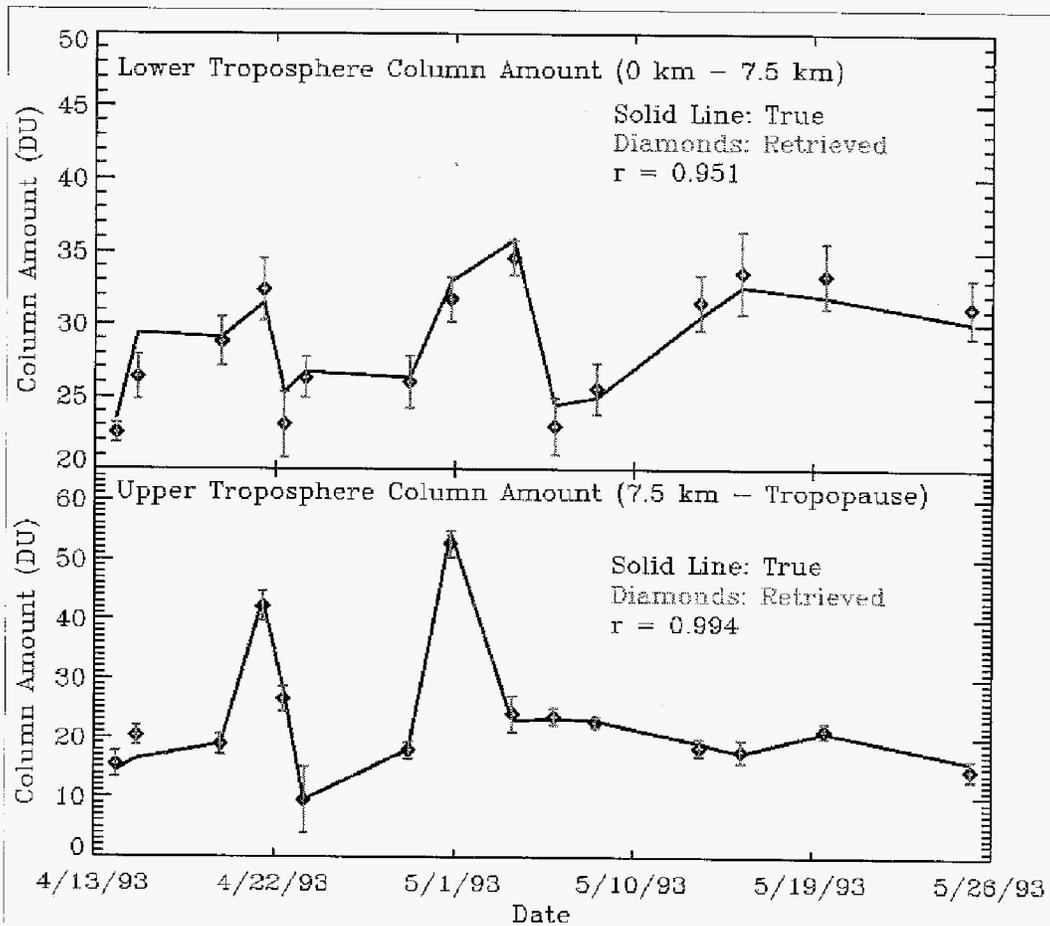


Fig 2. Time series of retrieved and true columns for the upper and lower troposphere for the Bermuda profiles.

Capturing Tropospheric Ozone Time Variability: A Study Using TES Nadir Retrieval Simulations

John Worden (Raytheon ITSS)

Kevin Bowman, Tilman Steck, and Helen Worden (JPL)

Tony Clough (AER)

Clive Rodgers (Oxford)

Talk Overview

- 1) (John) Initial guess refinement (IGR) validation
- 2) (Tilman) Level retrievals
 - i. Using diagonal S_a
 - ii. First derivative constraint
 - iii. Second derivative constraint
 - iv. climatology
- 3) (Kevin) Error analysis when X_a correlated with true profile
- 4) (John) Have we captured ozone time variability for this set of profiles?

Shape Retrieval: Is initial guess refinement robust?

Does IGR address the “large residual” problem?

- 1) IGR minimizes number of iterations to convergence.
- 2) Removes extraneous minima.
- 3) Refined initial guess is a small residual problem with respect to true solution.

Field-of-View Status

John Worden, Eugene Ustinov, Reggie Sakurai, Tony Clough, and Patrick Brown

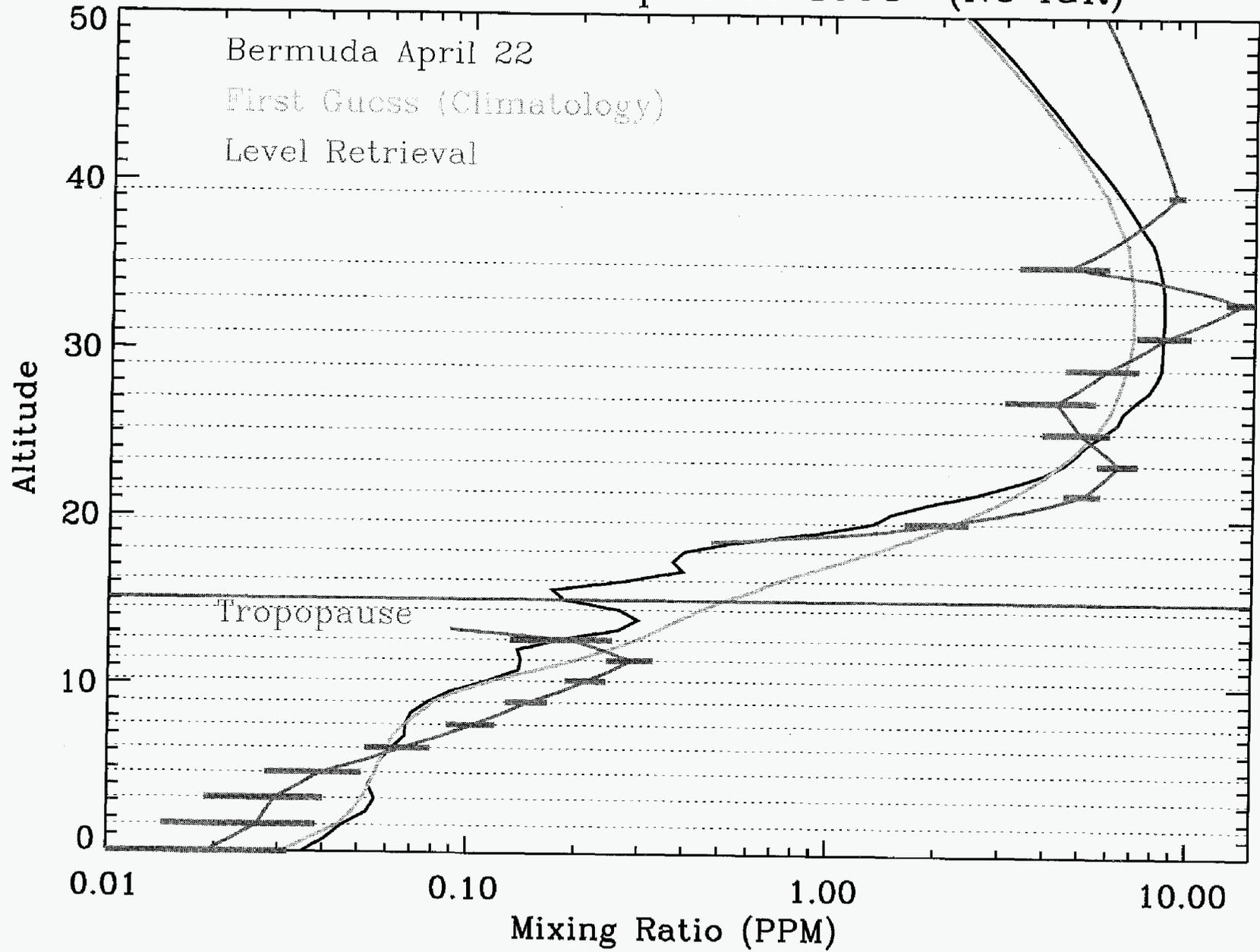
Issues from previous FOV code

- Hard-wired Gaussian FOV function
- Artificial surface rays
- Limited set of rays per detector
- Indexing problems associated with mapping and ray tracking
- Assumed uniform angular grid for rays entering detector

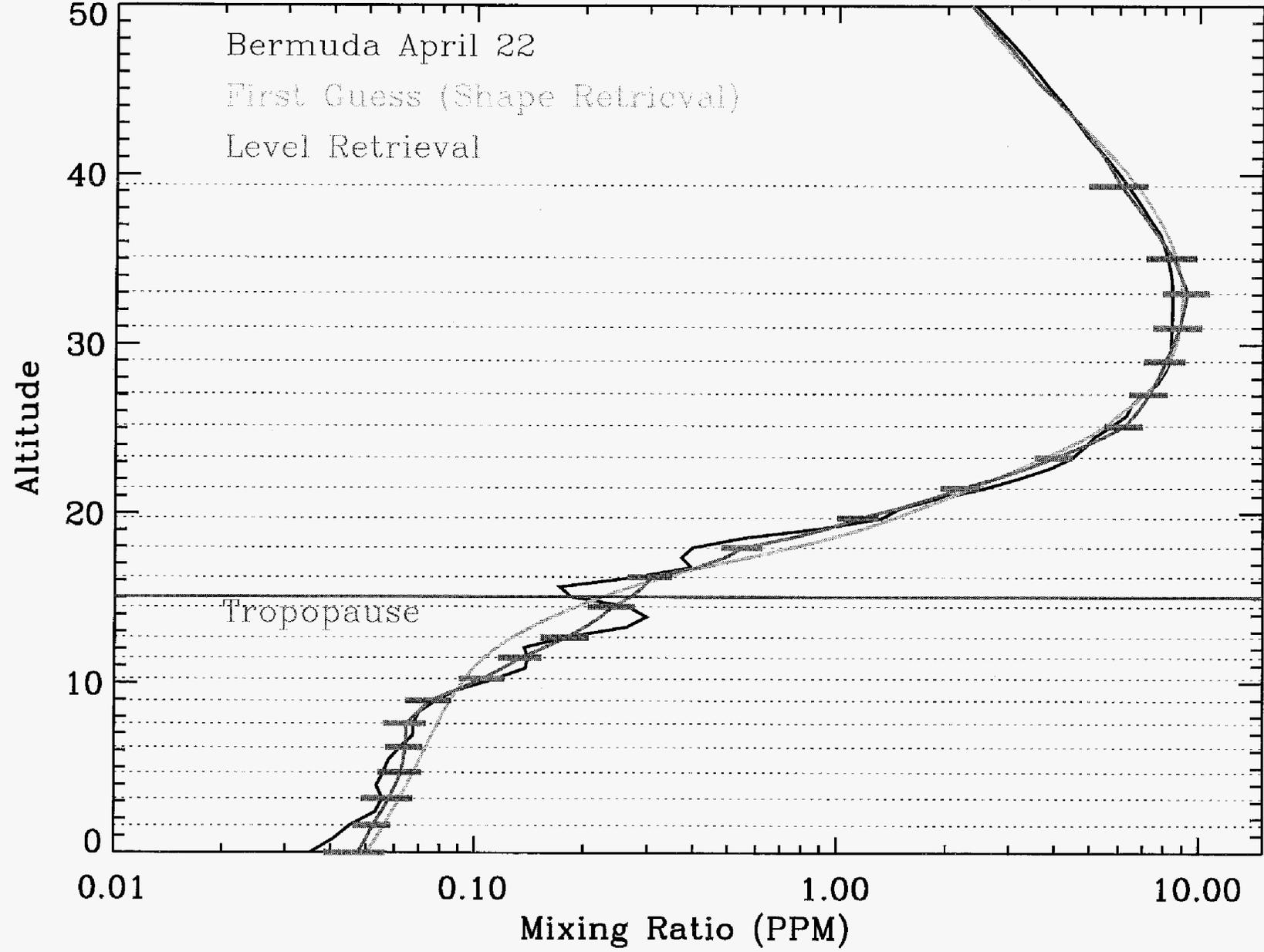
Current Status

- All rays enter all detectors.
 - This approach is still cheap because FM rays have to be computed anyways!
 - No mapping of rays to detectors; thus current code is much more compact.
- FOV function read from file
- All rays and corresponding satellite nadir angles must be pre-computed
 - Option to truncate, extrapolate, or re-normalize FOV function.
- Code is optimized for minimizing CPU time. Primary summation is over ray index.
- Four-point interpolation (with continuous derivatives) assumes non-uniform ray and FOV grid.

Bermuda Ozone April 22 1993 (No IGR)



Bermuda Ozone April 22 1993 (IGR = Shape Retrieval)



Result Overview

Results of the Bermuda retrievals. Considered altitude range for calculating the mean values is 1000.0 mbar - 10.0 mbar.

| Date | rel. rms [%] | max. dev. [%] ([km]) | abs. rms [ppm] | max. dev. [ppm] ([km]) | vert. res. [km] | dfs |
|----------|-----------------|-------------------------|-------------------|---------------------------|--------------------|-------------|
| April 14 | 16.7 | 52.3 (12.5) | 0.348 | 0.967 (22.6) | 6.21 | 7.59 |
| April 15 | 21.9 | 71.5 (14.1) | 0.221 | 0.604 (26.2) | 6.98 | 7.40 |
| April 19 | 13.4 | 72.9 (65.8) | 0.206 | 0.590 (25.1) | 6.70 | 7.42 |
| April 21 | 16.9 | 43.1 (12.0) | 0.273 | 1.11 (35.1) | 6.39 | 7.63 |
| April 22 | 19.7 | 68.7 (13.9) | 0.224 | 0.759 (29.0) | 6.82 | 7.50 |
| April 23 | 18.7 | 58.8 (14.4) | 0.147 | 0.837 (33.0) | 6.95 | 7.46 |
| April 28 | 18.0 | 45.7 (13.2) | 0.283 | 0.791 (32.4) | 6.24 | 7.78 |
| April 30 | 23.9 | 49.2 (12.6) | 0.259 | 1.28 (35.1) | 6.22 | 7.96 |
| May 3 | 15.0 | 45.8 (5.39) | 0.326 | 1.26 (25.7) | 6.53 | 7.64 |
| May 5 | 12.1 | 36.2 (17.9) | 0.221 | 0.993 (31.3) | 6.40 | 7.71 |
| May 7 | 19.1 | 55.8 (13.7) | 0.224 | 0.578 (39.5) | 6.51 | 7.62 |
| May 12 | 8.37 | 26.9 (6.87) | 0.173 | 0.964 (35.3) | 6.10 | 7.90 |
| May 14 | 22.3 | 55.7 (13.9) | 0.185 | 0.564 (35.3) | 6.51 | 7.74 |
| May 18 | 14.8 | 44.2 (12.1) | 0.220 | 1.35 (33.2) | 6.75 | 7.59 |
| May 25 | 11.1 | 72.6 (65.9) | 0.178 | 0.518 (31.1) | 6.66 | 7.58 |

Constraints

- (1) $\mathbf{R} = \mathbf{S}_a^{-1}$ (**diagonal matrix**), where the diagonal is 30 % of the *a priori* profile, based on the estimate of the shape retrieval accuracy.
- (2) $\mathbf{R} = \alpha \mathbf{L}^T \mathbf{L}$, where \mathbf{L} is the discrete **first derivative** operator.
- (3) $\mathbf{R} = \alpha \mathbf{L}^T \mathbf{L}$, where \mathbf{L} is the discrete **second derivative** operator. $\mathbf{L}^T \mathbf{L}$ is normalized to the logarithm of pressure and the strength (α) is chosen so that the degrees of freedom (trace of the averaging kernel) is about 9.
- (4) $\mathbf{R} = \mathbf{S}_a^{-1}$, where \mathbf{S}_a is from **climatology**. The retrieval parameters are the logarithm of the vmr profile and Levenberg-Marquardt is used.

For the cases (1) - (3) the initial guess and *a priori* profiles are equal to shape retrieval results whereas a climatology profile is used in case (4).

Constraints cont.

First derivative constraint:

- Purpose: smoothing the solution profile without shifting it towards the *a priori* profile.
- Operator

$$\mathbf{L} = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & \vdots \\ \vdots & \dots & \dots & \dots & 0 \\ 0 & \dots & 0 & -1 & 1 \end{pmatrix} \quad (1)$$

leads to

$$\mathbf{L}^T \mathbf{L} = \begin{pmatrix} 1 & -1 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & \vdots \\ 0 & \dots & \dots & \dots & \dots & \vdots \\ \vdots & \dots & \dots & \dots & \dots & 0 \\ \vdots & \dots & 0 & -1 & 2 & -1 \\ 0 & \dots & \dots & 0 & -1 & 1 \end{pmatrix}. \quad (2)$$

- $(\mathbf{x} - \mathbf{x}_a)^T \alpha \mathbf{L}^T \mathbf{L} (\mathbf{x} - \mathbf{x}_a)$ minimizes an **absolute** distance (smoothing) between the retrieved and the *a priori* profile.
 - relatively strong constraint near ozone maximum
 - relatively weak constraint in troposphere

Constraints cont.

- Scaling the constraint matrix with the inverse of the *a priori* profile

$$\mathbf{B}^{-1} = \begin{pmatrix} \frac{1}{x_a^1} & 0 & \cdots & 0 \\ 0 & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & 0 \\ 0 & \cdots & 0 & \frac{1}{x_a^n} \end{pmatrix}. \quad (3)$$

Therefore we receive $\alpha \mathbf{B}^{-1} \mathbf{L}^T \mathbf{L} \mathbf{B}^{-1}$ which constrains relative values $\left(\frac{x^i - x_a^i}{x_a^i}\right)$.

- Determine total strength of constraint by calculating α iteratively that the following condition is met:

$$\frac{1}{p} \sum_{i=1}^p \frac{\sigma_i}{x_a^i} = \frac{1}{p} \sum_{i=1}^p \frac{\sqrt{S_{ii}}}{x_a^i} \approx 20\%, \quad (4)$$

σ , standard deviation,

p , number of considered levels (in our case between 1000.0 and 10.0 mbar),

$$\mathbf{S} = (\mathbf{K}_0^T \mathbf{S}_\epsilon^{-1} \mathbf{K}_0 + \alpha \mathbf{B}^{-1} \mathbf{L}^T \mathbf{L} \mathbf{B}^{-1})^{-1},$$

\mathbf{K}_0 , Jacobian evaluated at the initial guess profile \mathbf{x}_0 .

Conclusions

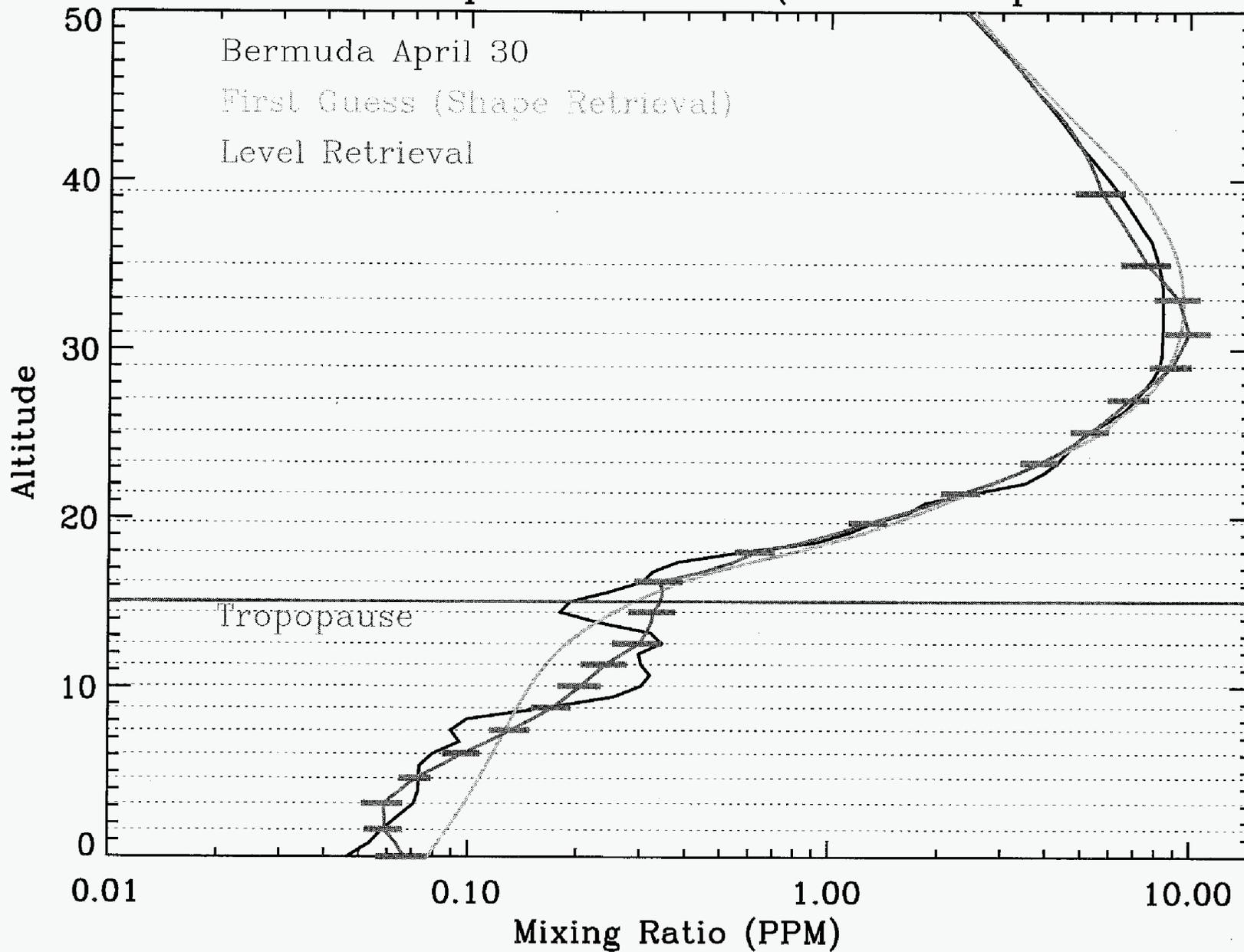
- Estimated TES vertical resolution is between 5 and 7 km in troposphere. Average total error is about 20 %.
- Diagonal S_a introduces structure (jack-knifing) below the expected TES vertical resolution.
- Smoothing constraints eliminate jack-knifing while retaining expected TES vertical resolution.
- Features can be captured that are larger than the TES vertical resolution.
- The smoothing constraints gives the best results over the ensemble of profiles, where the first derivative constraint is slightly better than the second derivative.

Level Retrieval Comparison

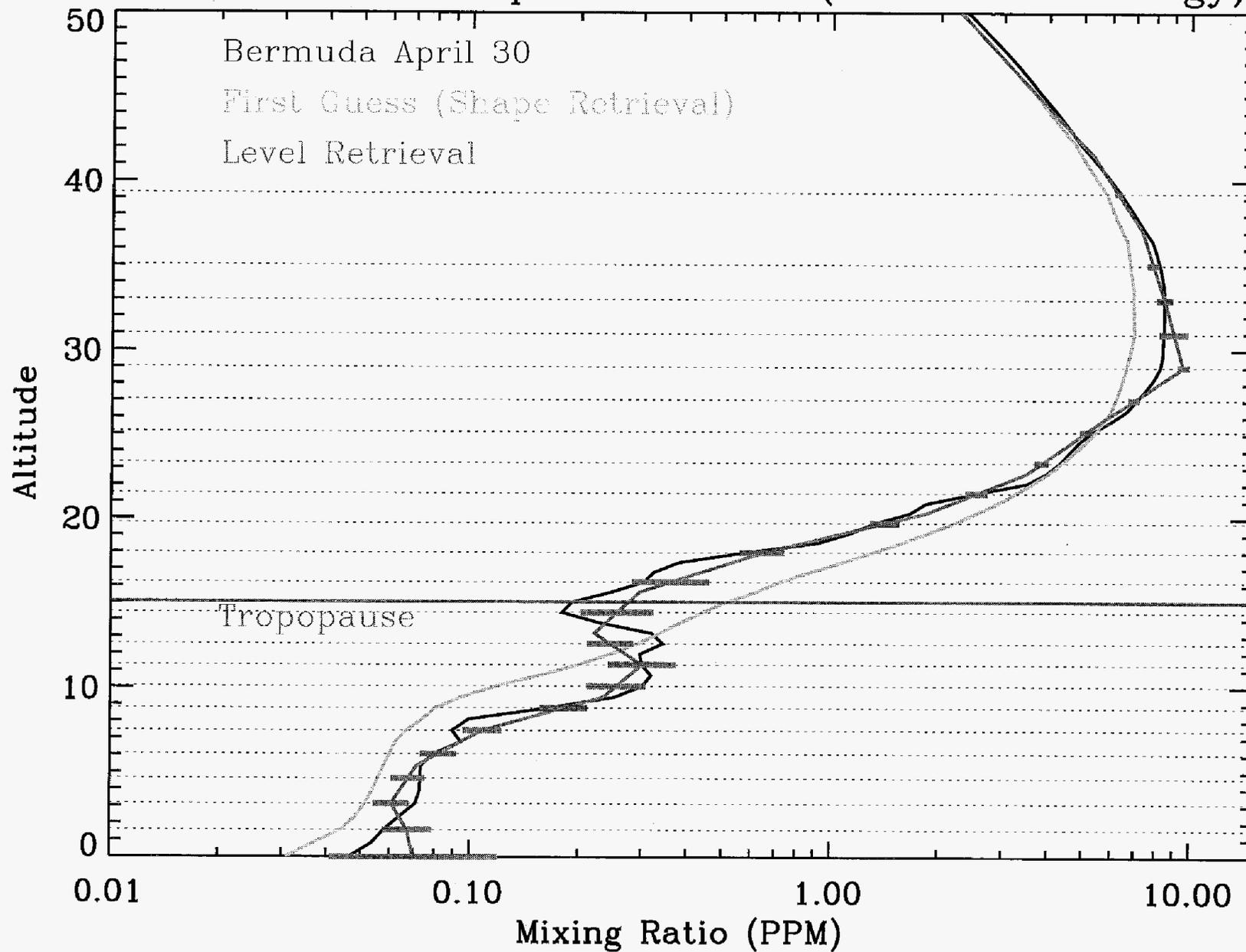
Overview:

- 15 ozone sonde data from the Bermuda station were taken between April 14, 1993 and May 25, 1993.
- Each measurement contain a set of temperature, water vapor, and ozone profiles.
- Signal-to-noise ratio (SNR) is set to 300 (NESR = $1.32 \times 10^{-8} \text{ W}/(\text{cm}^2 \text{ sr cm}^{-1})$).
- Considered spectral range for retrieval: 985.0 - 1075.0 cm^{-1} .
Spectral resolution: 0.06 cm^{-1} .
- Assumption that surface temperature, atmospheric temperature, and water vapor are known.
- Number of forward model levels: 85.
Number of retrieval levels: 26.
- Retrieval results were calculated assuming different *a priori* and initial guess profiles as well as different constraint matrices \mathbf{R} in $\|\mathbf{x} - \mathbf{x}_a\|_{\mathbf{R}}^2$.

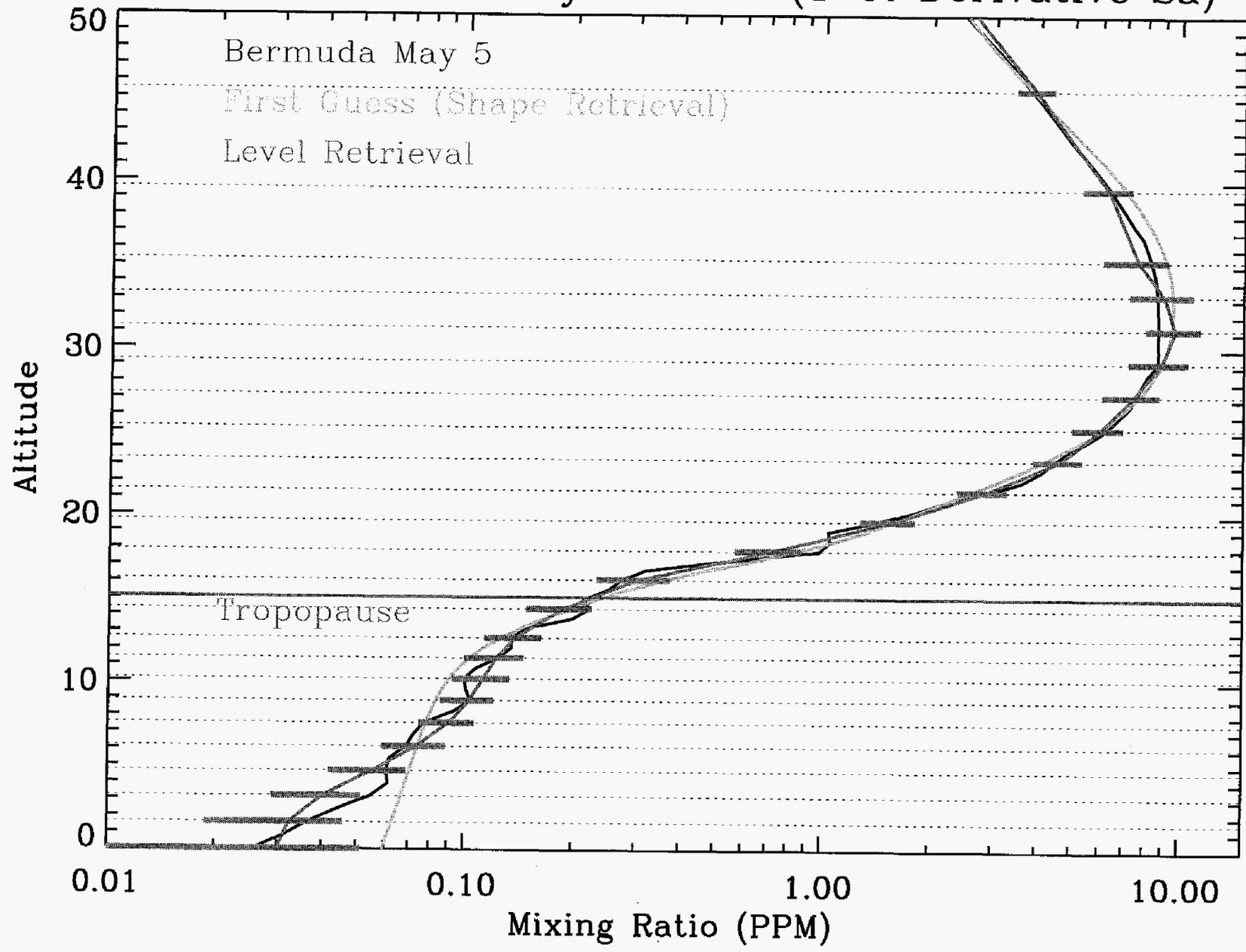
Bermuda Ozone April 30 1993 (IGR = Shape Retrieval)



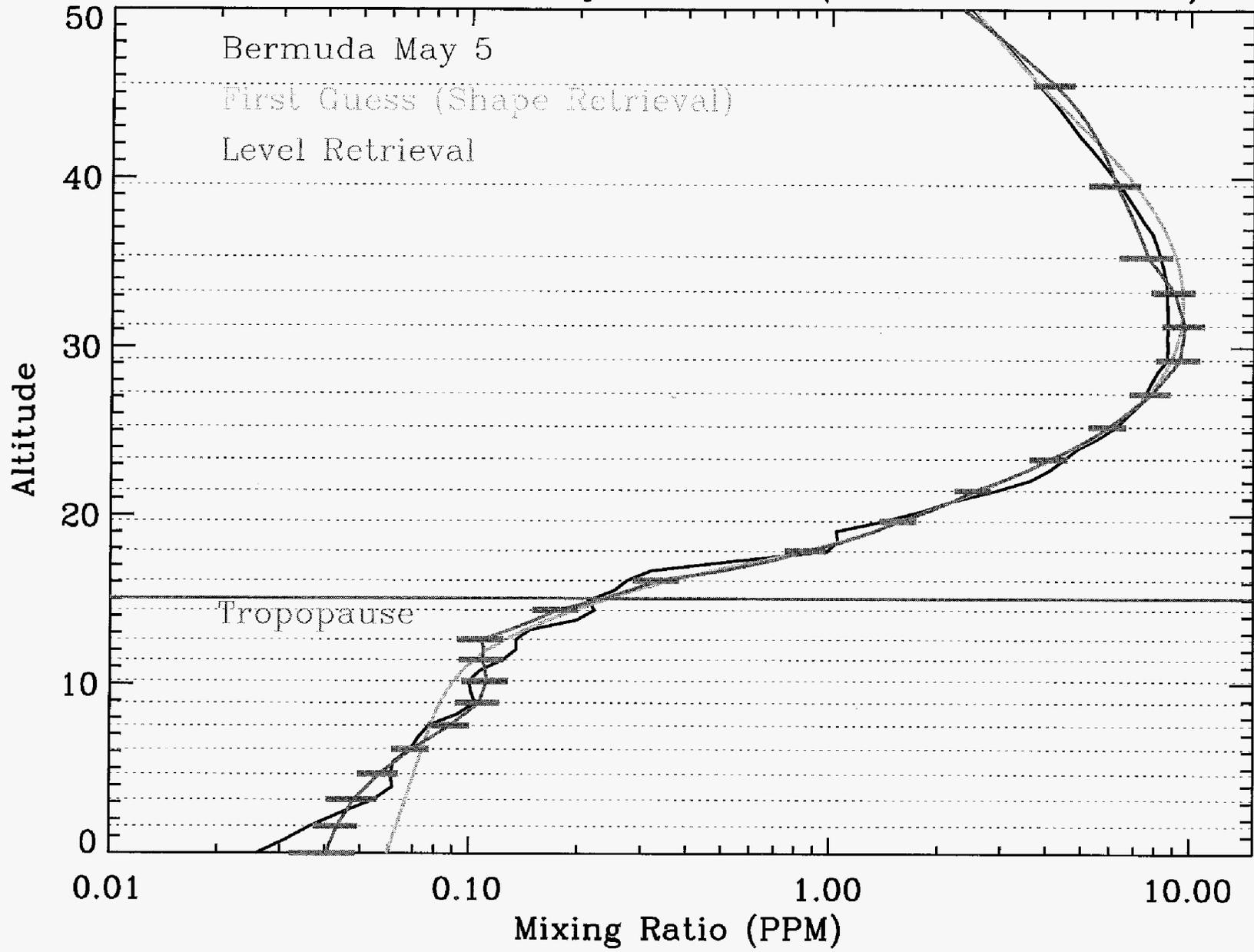
Bermuda Ozone April 30 1993 (IGR = Climatology)



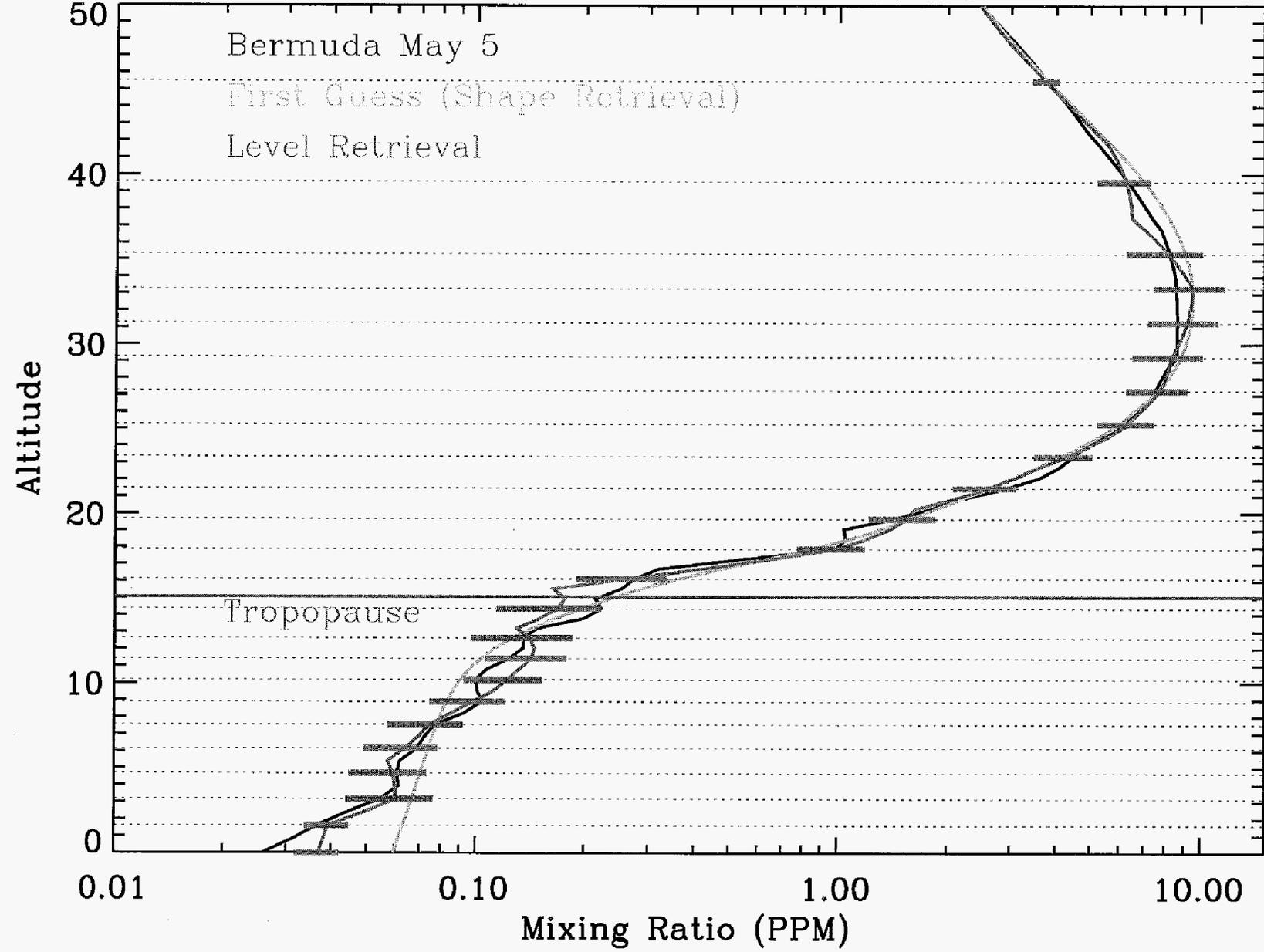
Bermuda Ozone May 5 1993 (1stst Derivative Sa)



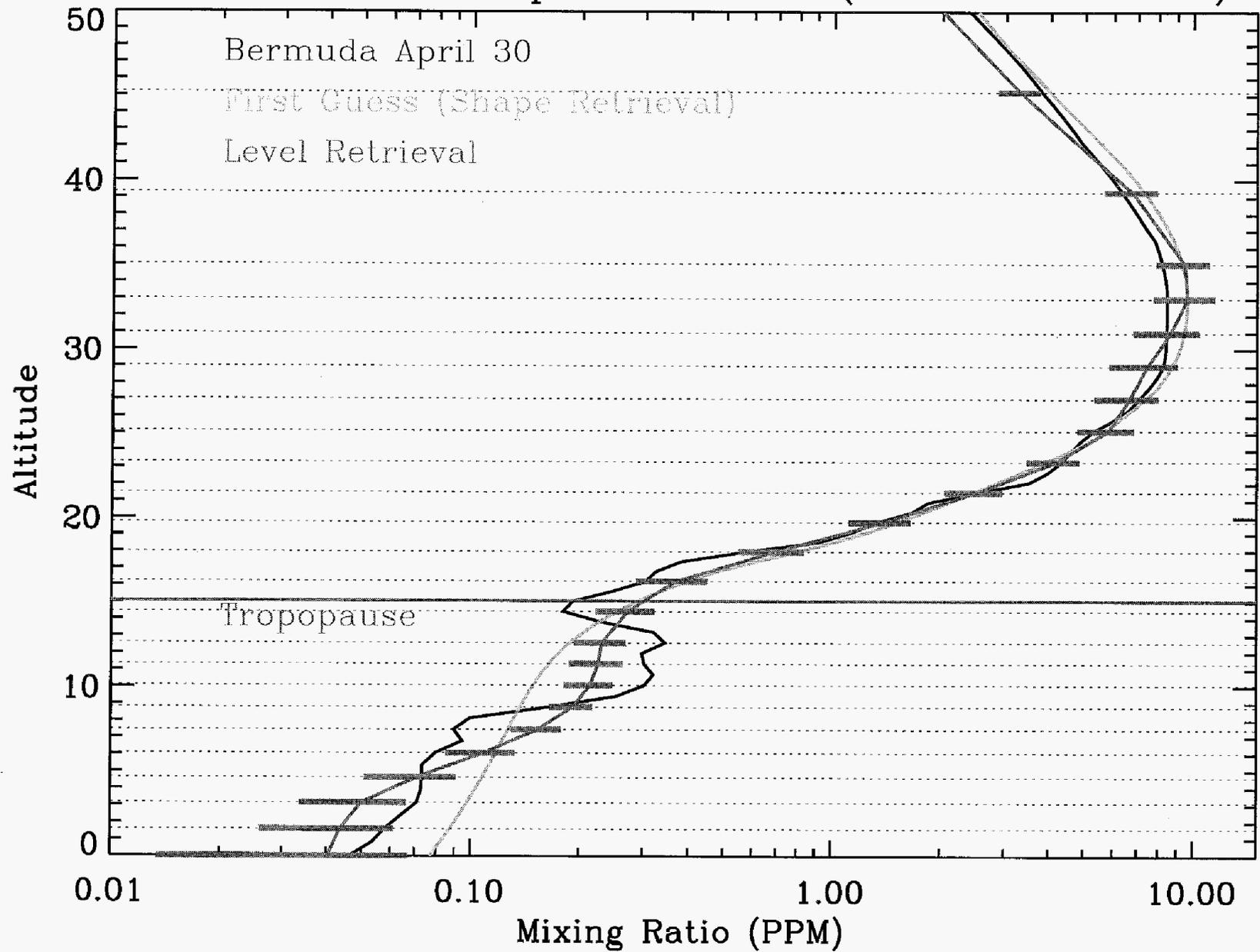
Bermuda Ozone May 5 1993 (2nd Derivative Sa)



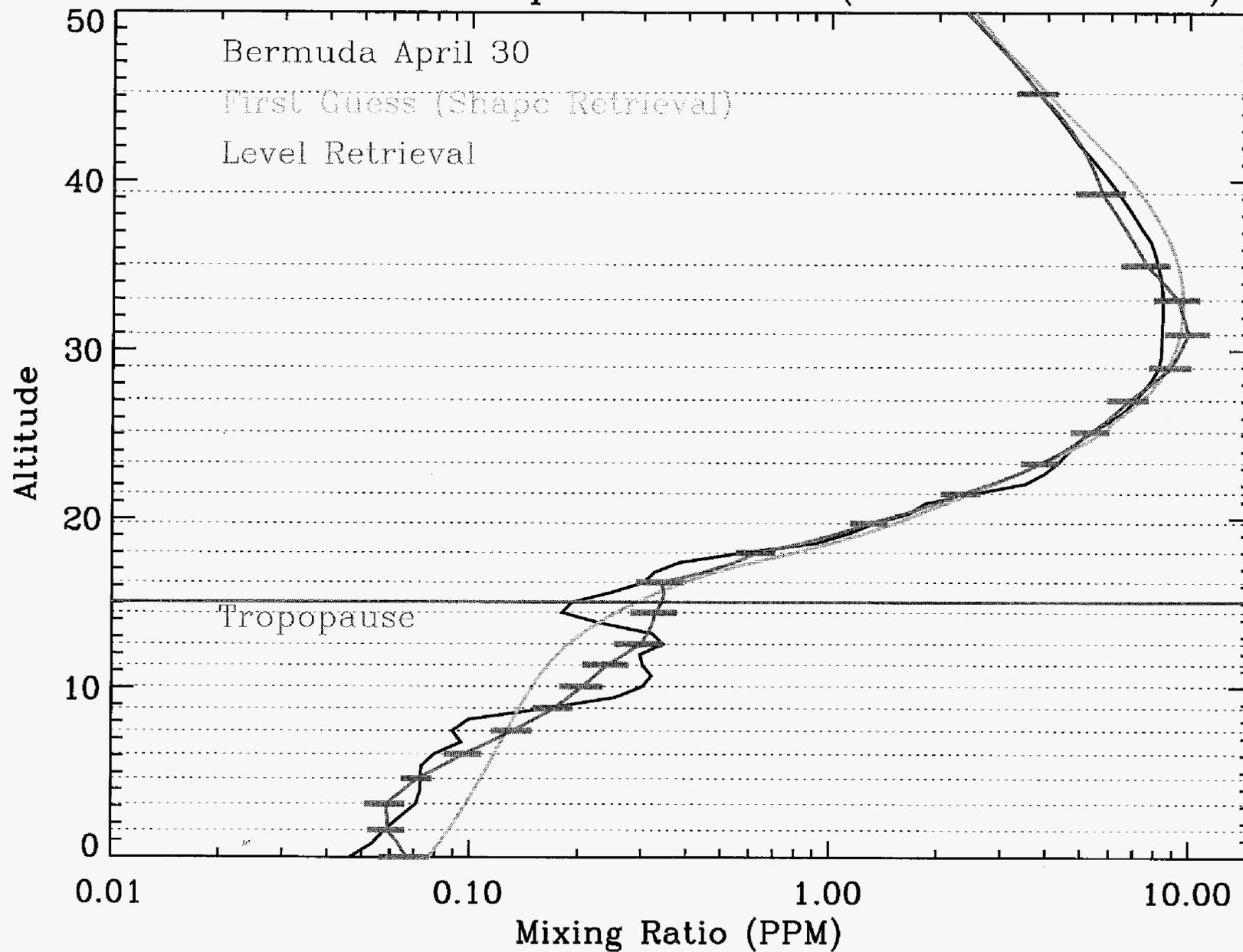
Bermuda Ozone May 5 1993 (Diagonal Sa)



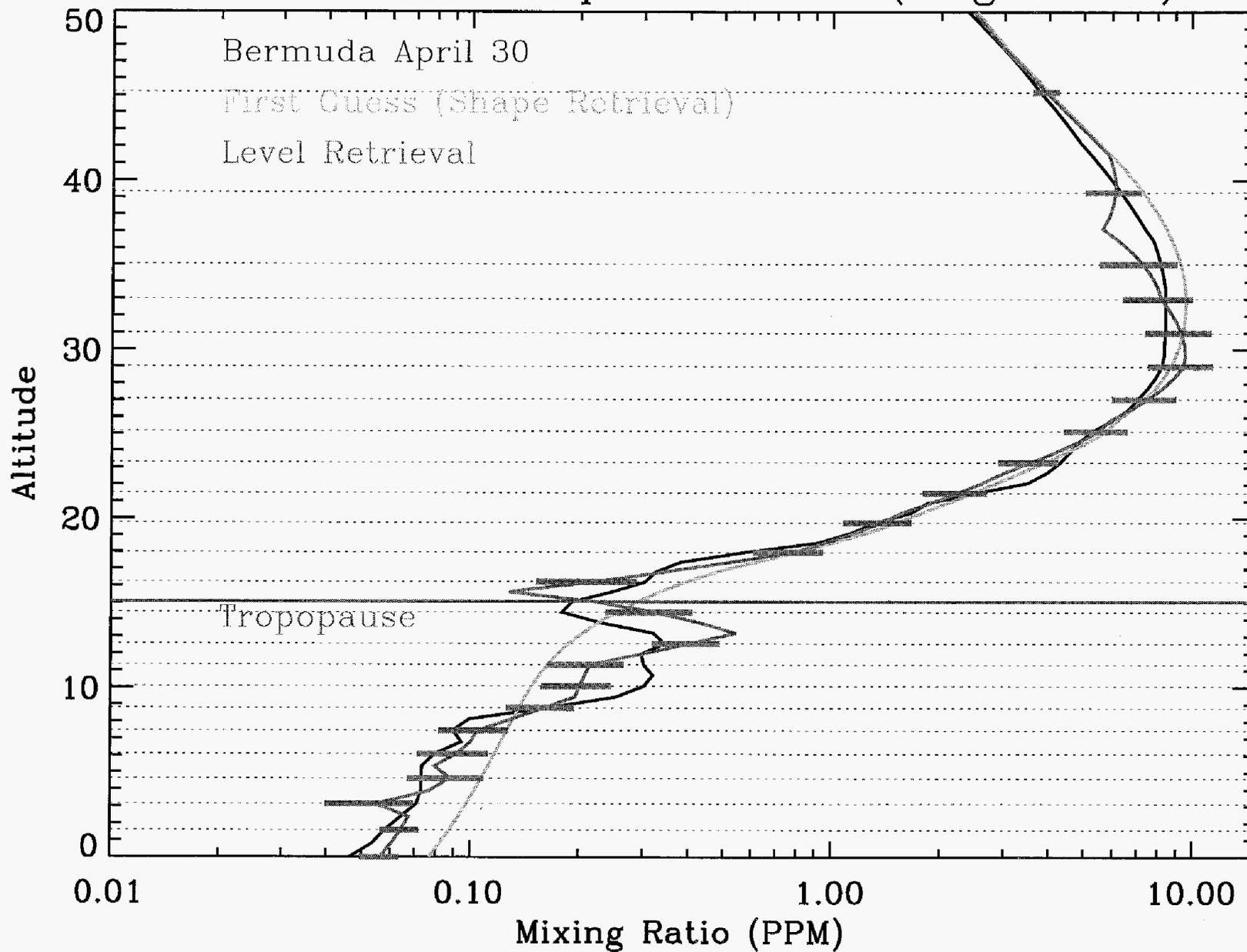
Bermuda Ozone April 30 1993 (1st Derivative Sa)



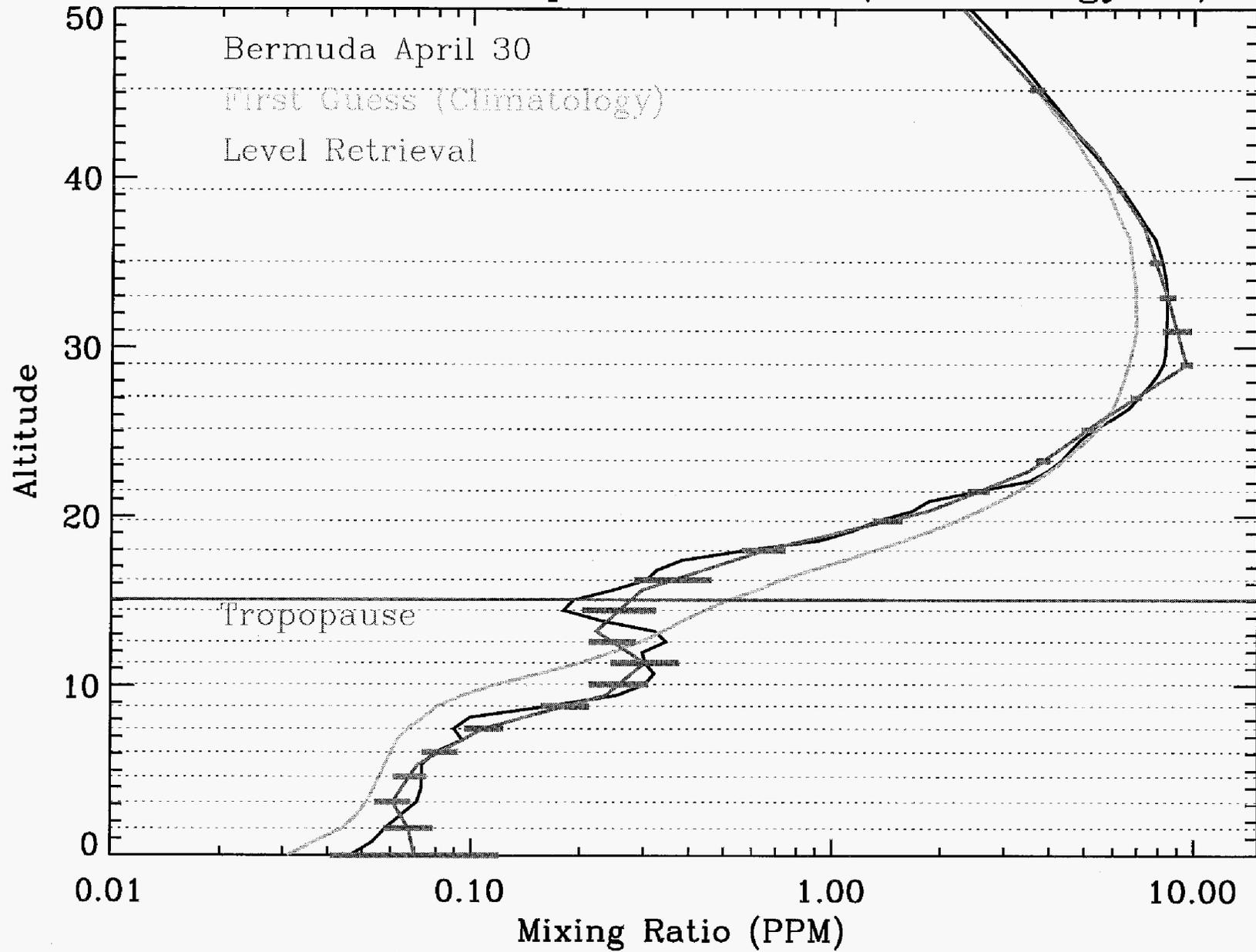
Bermuda Ozone April 30 1993 (2nd Derivative Sa)



Bermuda Ozone April 30 1993 (Diagonal Sa)



Bermuda Ozone April 30 1993 (Climatology Sa)



Major Thrust of the Error Analysis

- Extend classical error analysis techniques to address a 2-step retrieval method.
 - Compare theoretical and empirical calculations of error terms.
-

Linear estimate of retrieval

A linear estimate of retrieval is

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}_{xx}^z(\mathbf{x} - \mathbf{x}_a) + \mathbf{M}\mathbf{G}_z\epsilon$$

where $\mathbf{x}_a = \mathbf{M}\mathbf{z}_a$ is the a priori state vector and the averaging kernel on the forward model (FM) levels is $\mathbf{A}_{xx}^z = \mathbf{M}\mathbf{G}_z\mathbf{K}_x$. The mapping matrix is \mathbf{M} , the Jacobian on FM levels is \mathbf{K}_x , ϵ is noise, and the gain matrix is

$$\mathbf{G}_z = ((\mathbf{K}_x\mathbf{M})\mathbf{S}_\epsilon^{-1}(\mathbf{K}_x\mathbf{M})^\top + \Lambda)^{-1}(\mathbf{K}_x\mathbf{M})^\top\mathbf{S}_\epsilon^{-1}$$

Error analysis of linear estimate

The error in a single estimate is

$$\tilde{\mathbf{x}} = \hat{\mathbf{x}} - \mathbf{x} = \underbrace{(\mathbf{A}_{xx}^z - \mathbf{I})}_{\text{Smoothing error}} (\mathbf{x} - \mathbf{x}_a) + \underbrace{\mathbf{M}\mathbf{G}_z}_{\text{Noise error}} \epsilon,$$

The smoothing error is a function of the statistics of $\mathbf{x} - \mathbf{x}_a$ whereas the noise error is a function of the statistics of ϵ . For a fixed \mathbf{x}_a , the error covariance, $E((\tilde{\mathbf{x}} - \bar{\tilde{\mathbf{x}}})(\tilde{\mathbf{x}} - \bar{\tilde{\mathbf{x}}})^\top)$, over an ensemble of estimates is

$$\bar{\mathbf{S}} = \underbrace{(\mathbf{A}_{xx}^z - \mathbf{I})\mathbf{S}_e(\mathbf{A}_{xx}^z - \mathbf{I})^\top}_{\text{Smoothing error}} + \underbrace{\mathbf{M}\mathbf{G}_z\mathbf{S}_\epsilon(\mathbf{M}\mathbf{G}_z)^\top}_{\text{Noise error}},$$

where \mathbf{S}_e is the covariance of the true profiles on the FM grid and \mathbf{S}_ϵ is the covariance of the measurement noise.

Error analysis for 2 step retrieval

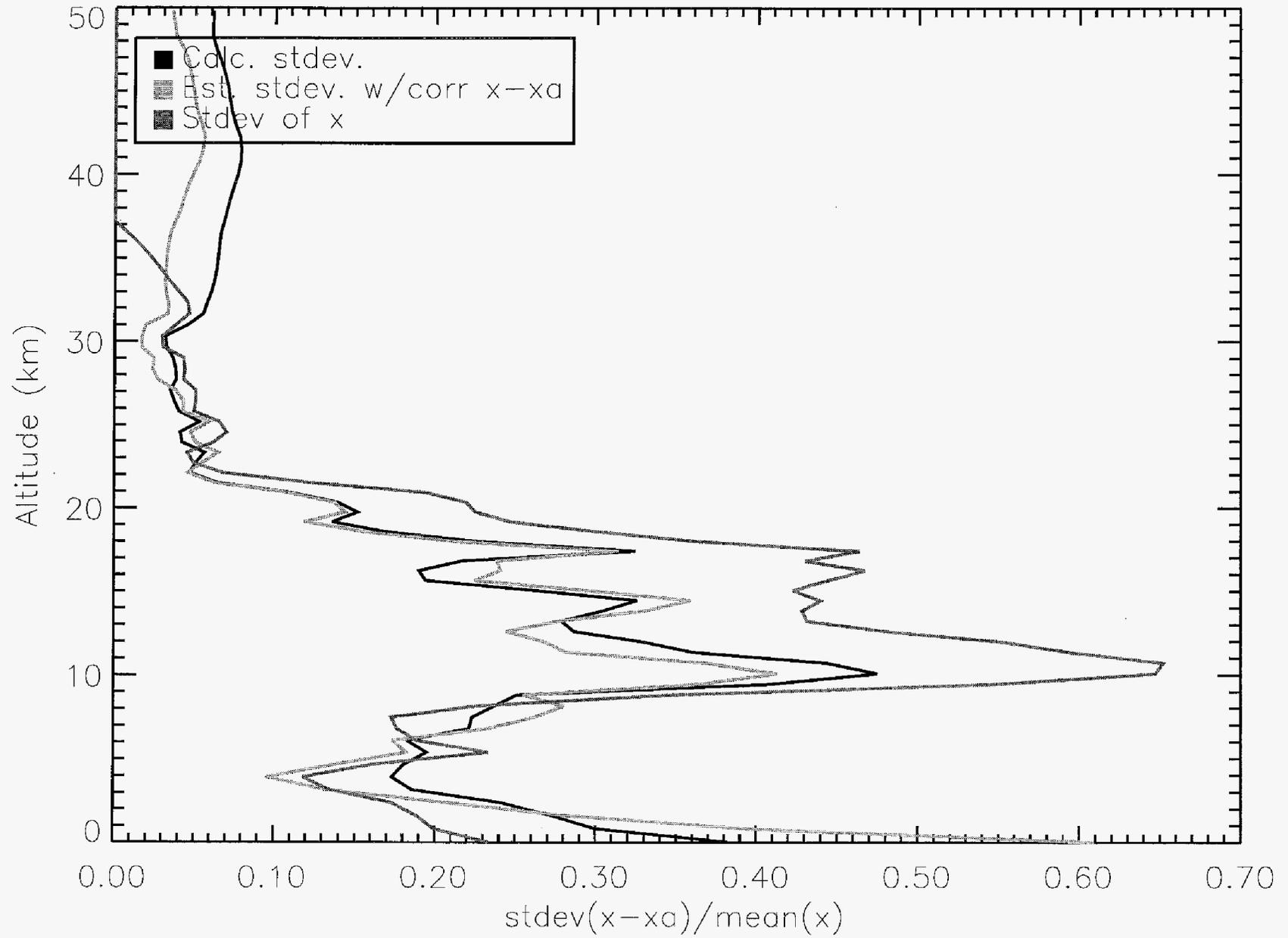
For our retrievals, the a priori state vector is an estimate of the true state that is calculated from the shape retrieval:

$$\mathbf{x}_a = \mathbf{x}_0 + \mathbf{A}_{xx}^s (\mathbf{x} - \mathbf{x}_0) + \mathbf{P}\mathbf{G}_s \epsilon,$$

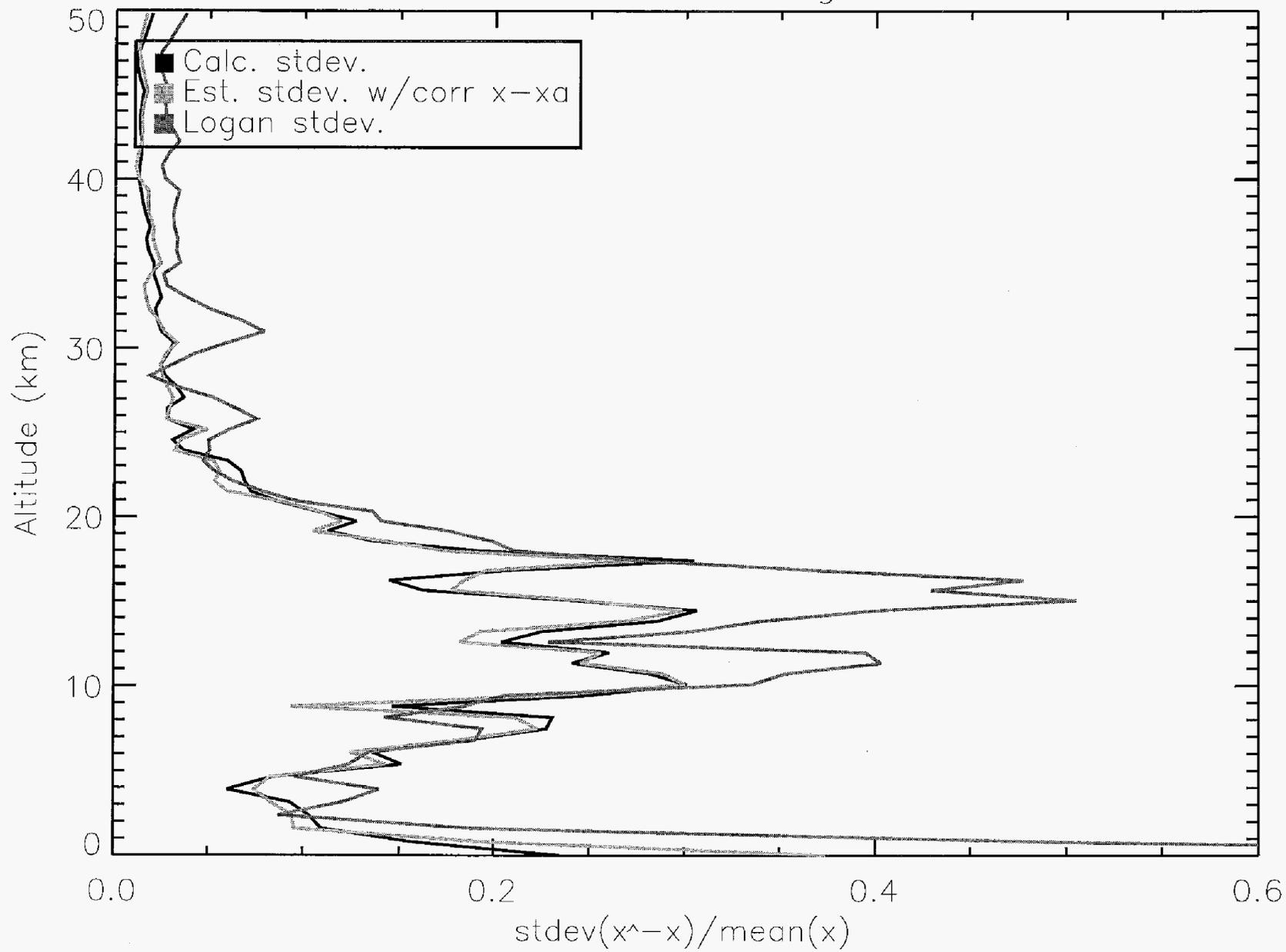
where \mathbf{x}_0 is the initial guess to the shape retrieval. Hence $\mathbf{x} - \mathbf{x}_a$ is the error in the estimate of the shape retrieval. The error in the estimate of the shape retrieval can be incorporated into the overall error:

$$\begin{aligned} \bar{\mathbf{S}} = & \underbrace{(\mathbf{A}_{xx}^z - \mathbf{I})(\mathbf{A}_{xx}^s - \mathbf{I})\mathbf{S}_e(\mathbf{A}_{xx}^s - \mathbf{I})^\top (\mathbf{A}_{xx}^z - \mathbf{I})^\top}_{\text{Smoothing error}} \\ & + \underbrace{((\mathbf{A}_{xx}^z - \mathbf{I})\mathbf{P}\mathbf{G}_s + \mathbf{M}\mathbf{G}_z)\mathbf{S}_\epsilon((\mathbf{A}_{xx}^z - \mathbf{I})\mathbf{P}\mathbf{G}_s + \mathbf{M}\mathbf{G}_z)^\top}_{\text{Noise error}}. \end{aligned}$$

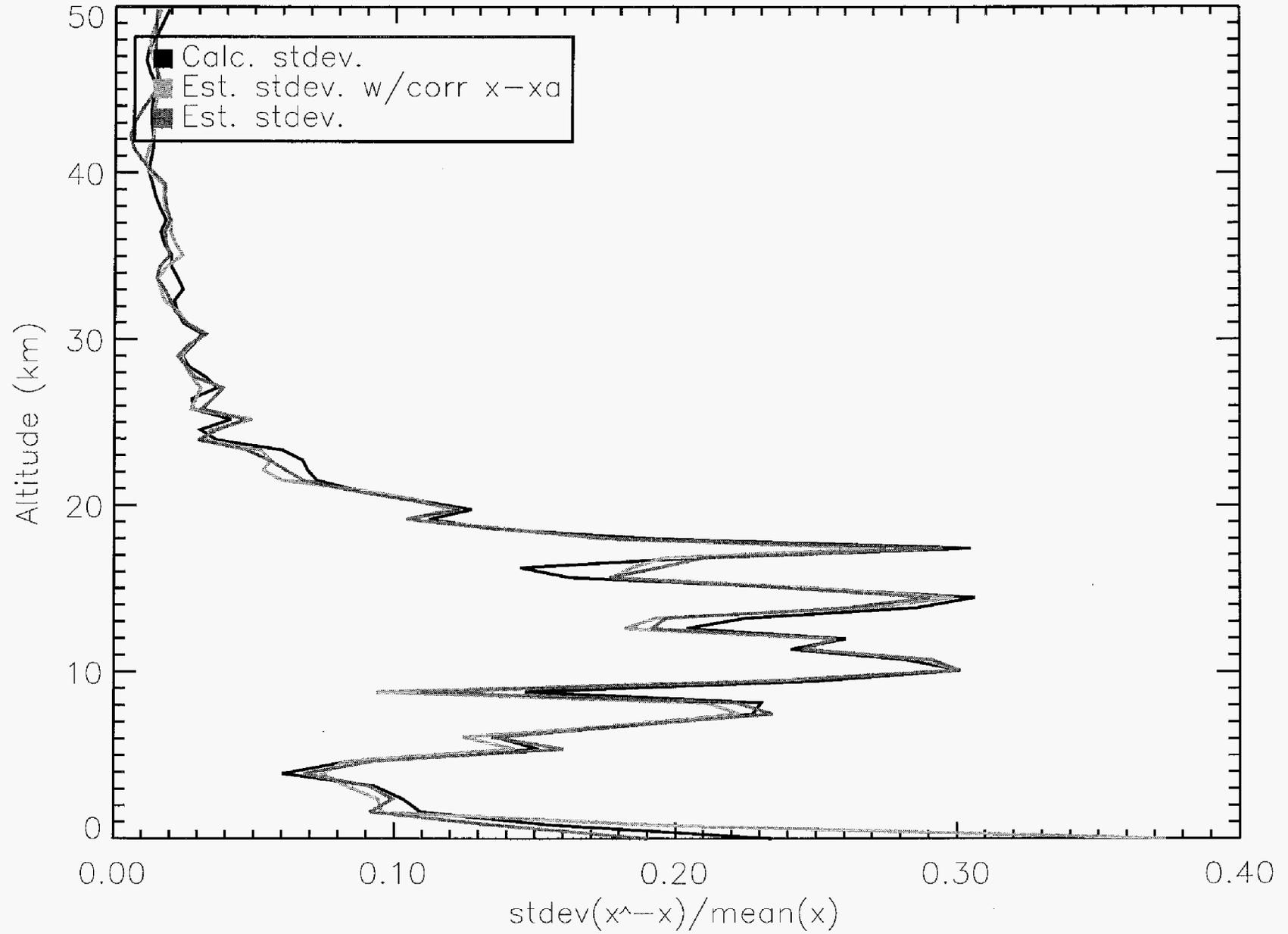
Fractional stdev of $x-x_a$



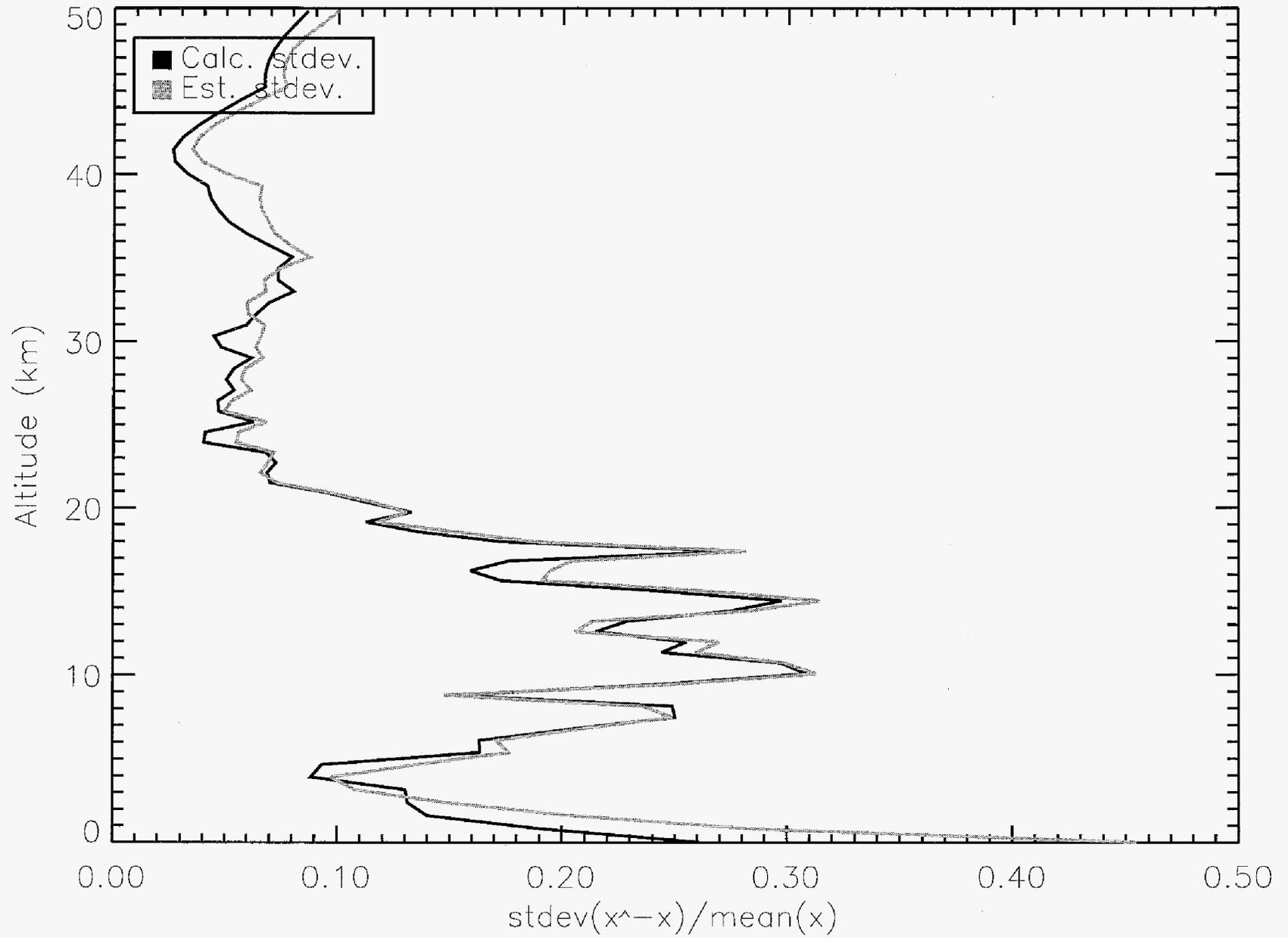
Fractional smoothing error



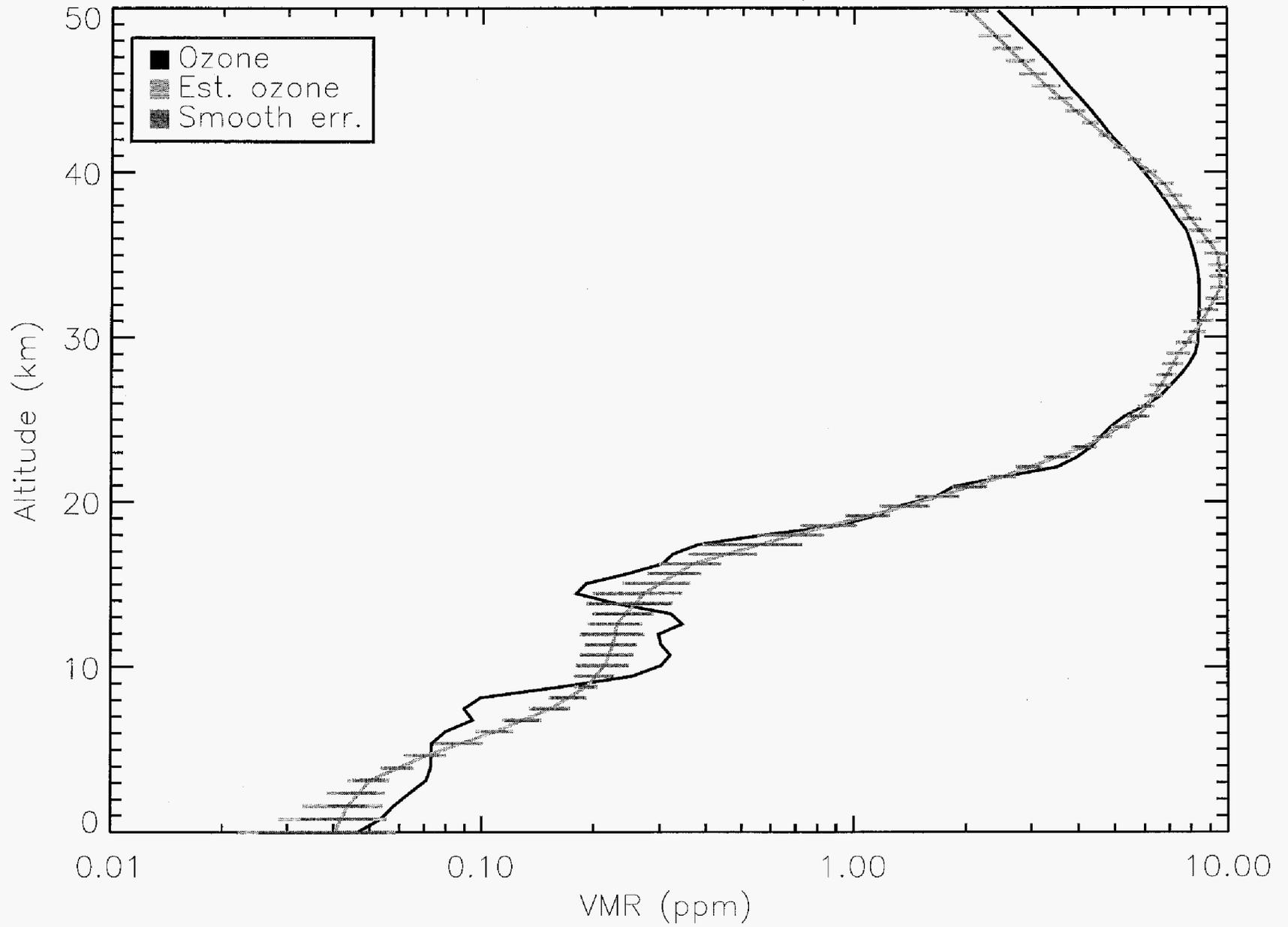
Fractional smoothing error



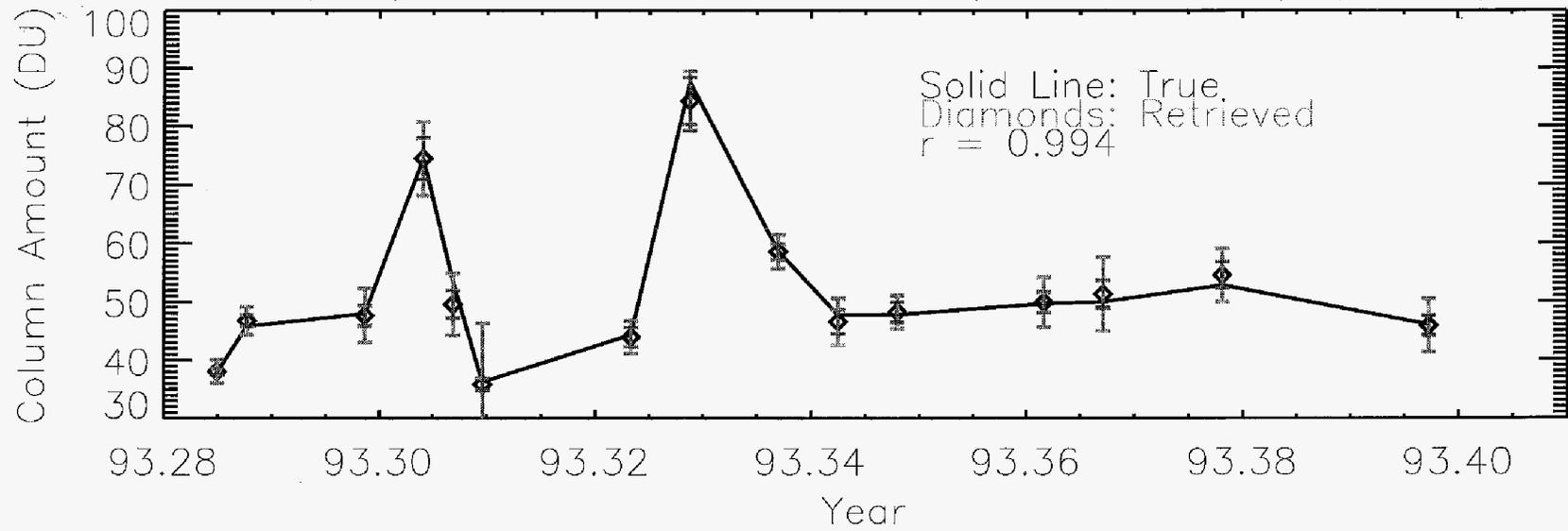
Fractional total error



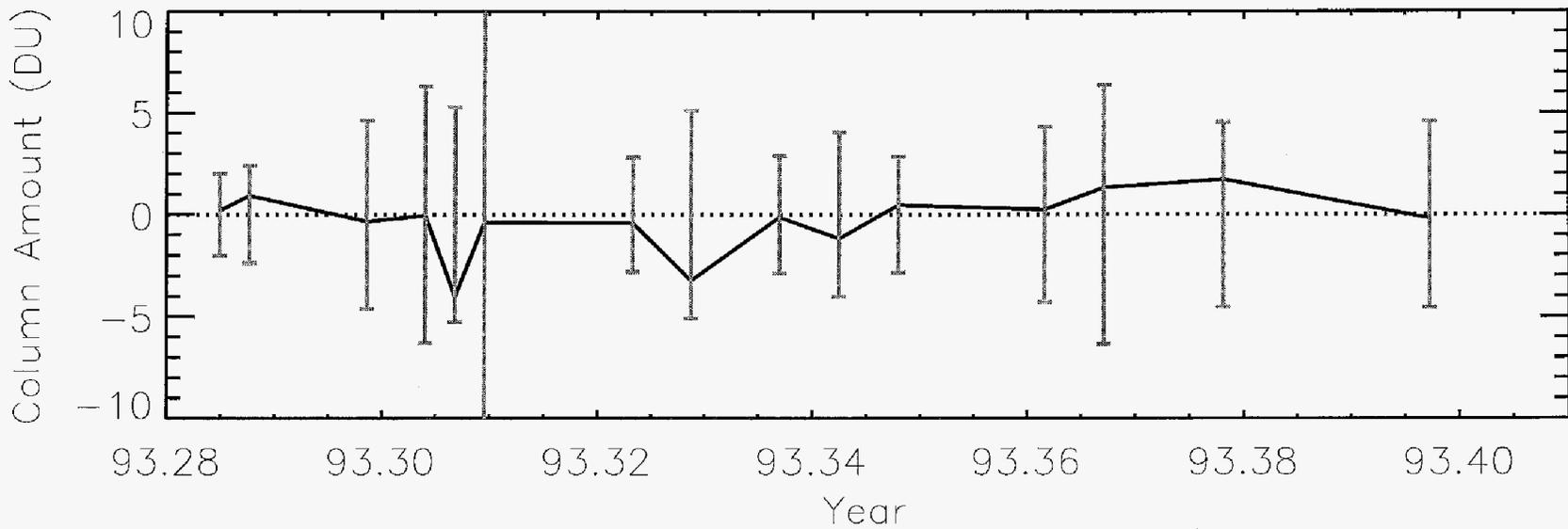
Ozone estimate of April 30.



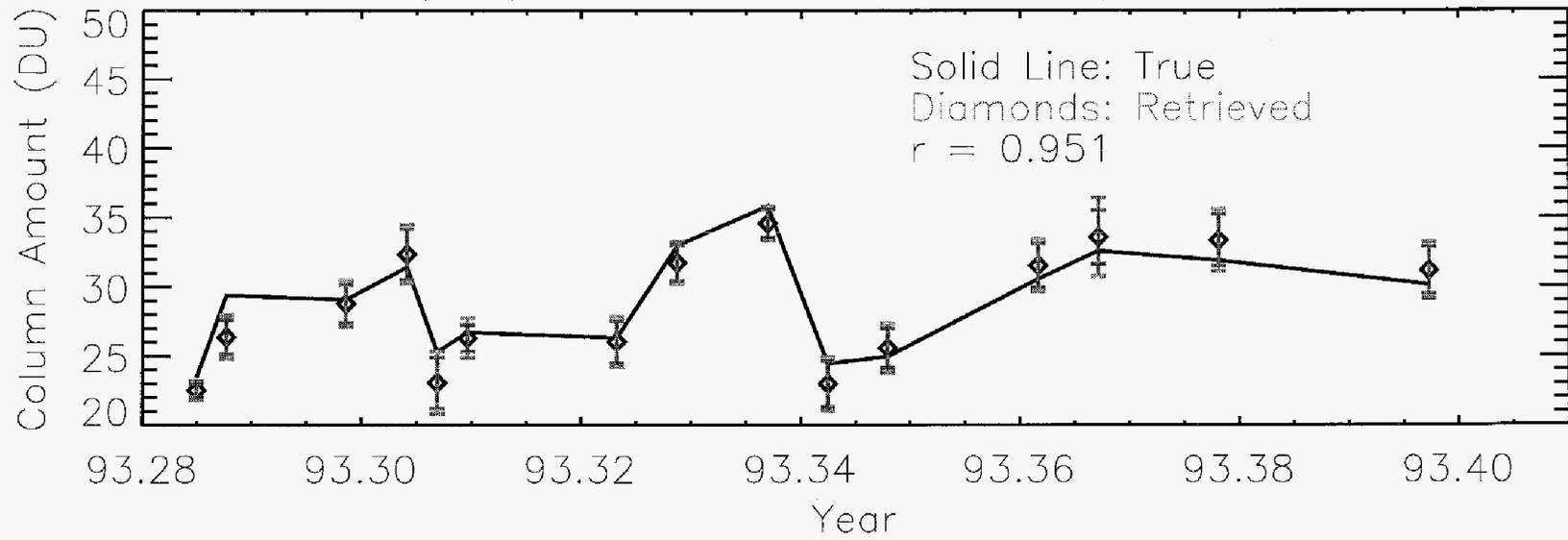
Troposphere Column Amount (0 km – Tropopause)



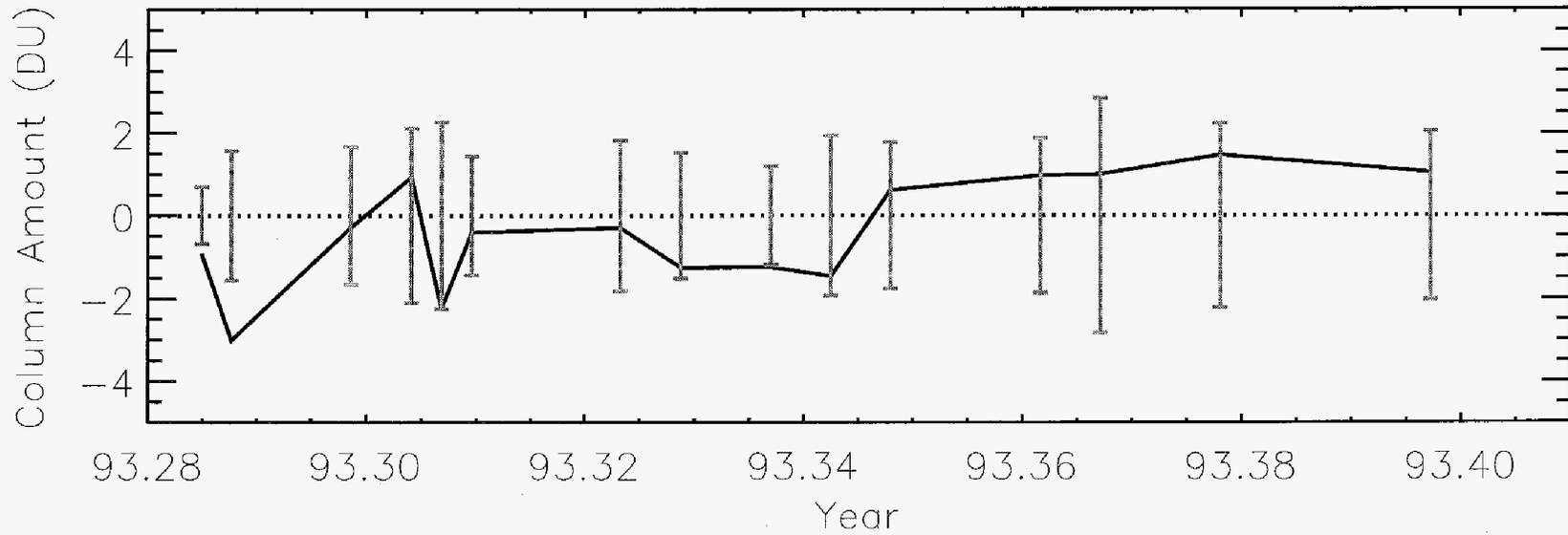
Retrieved – True



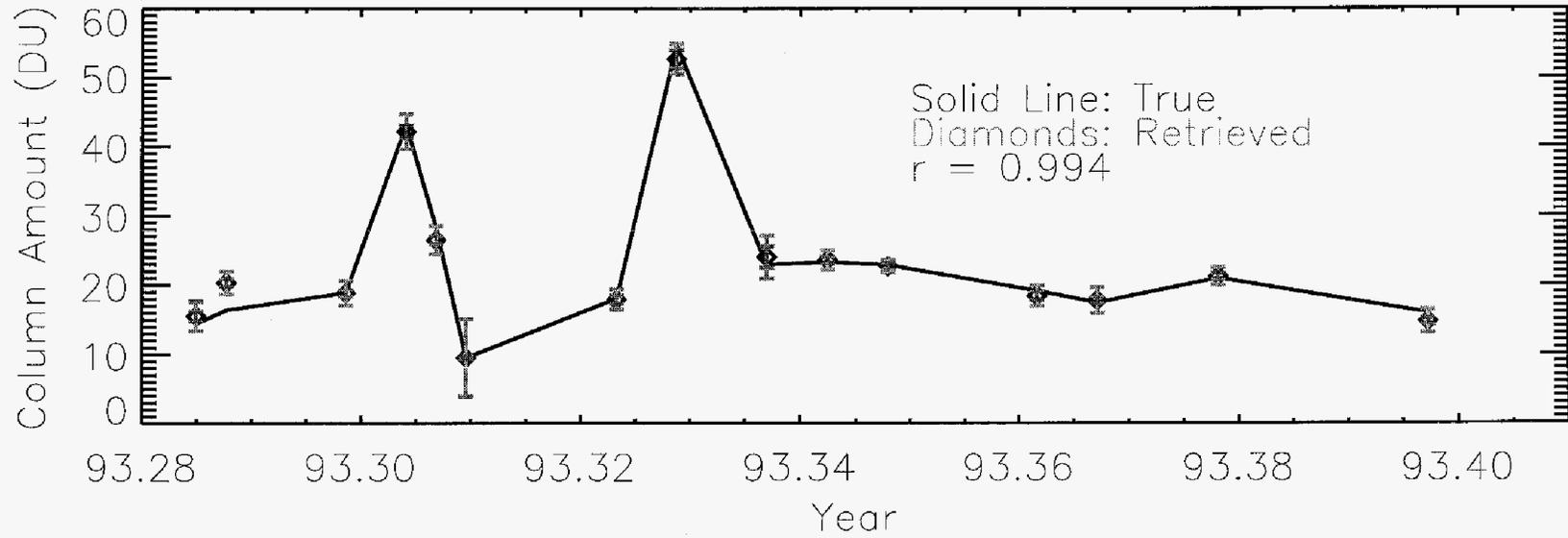
Lower Troposphere Column Amount (0 km – 7.5 km)



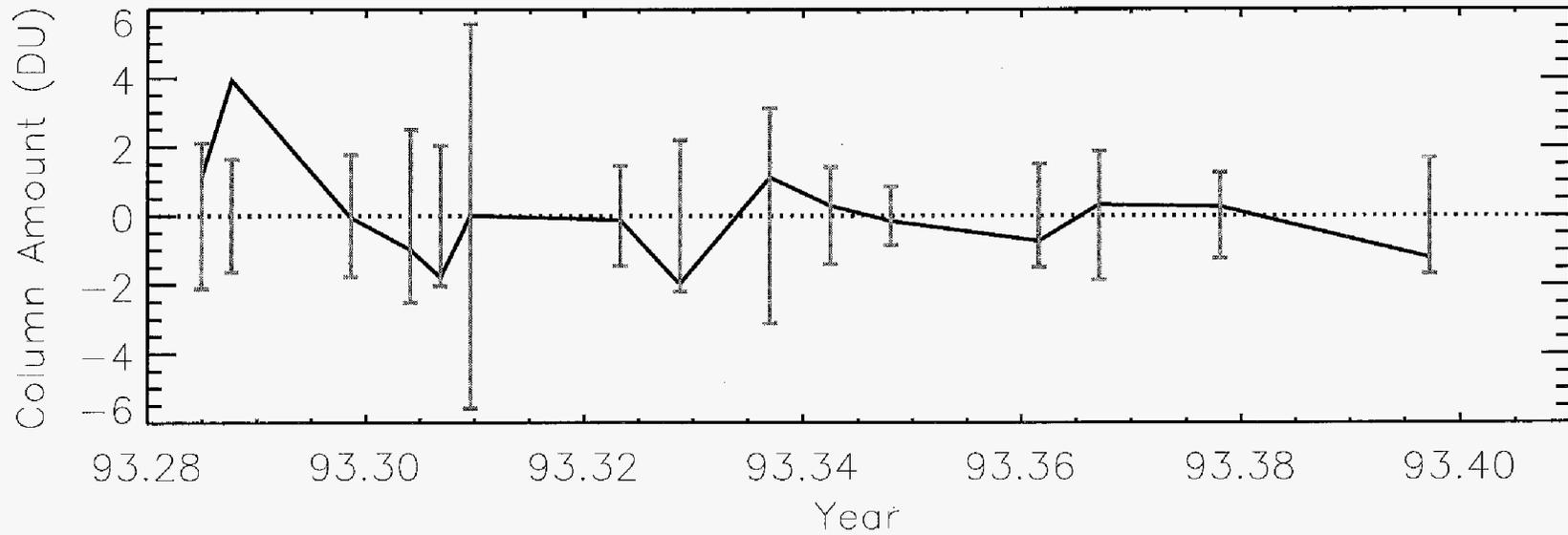
Retrieved – True



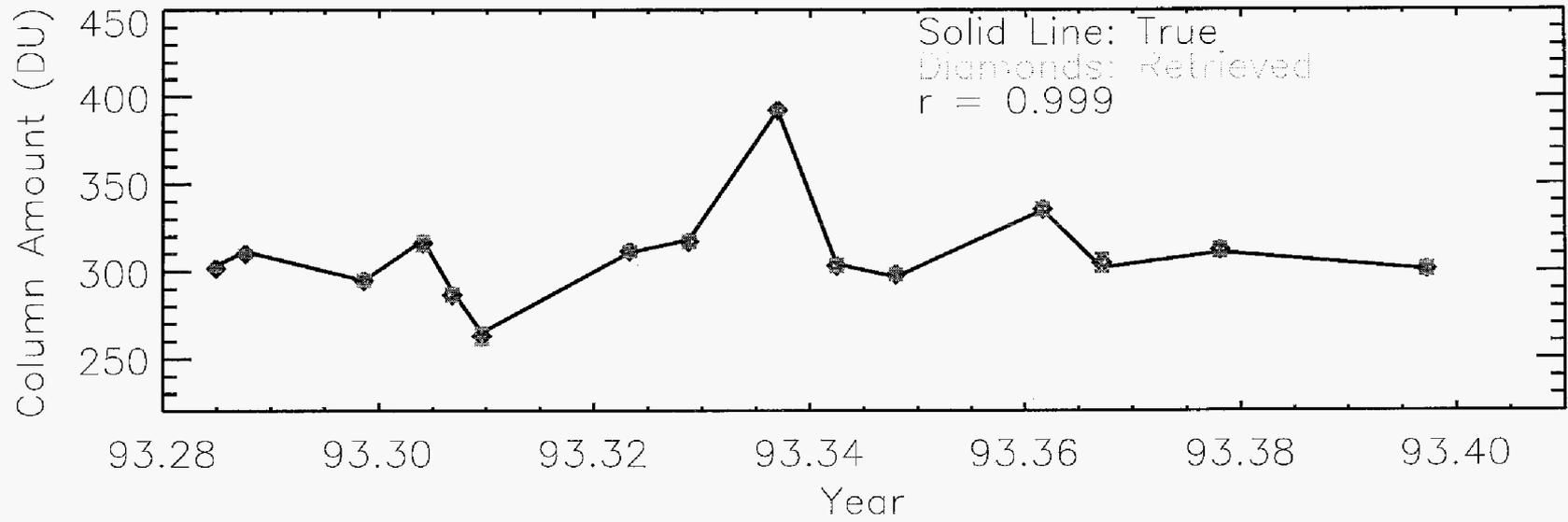
Upper Troposphere Column Amount (7.5 km – Tropopause)



Retrieved – True



Total Column Amount



Retrieved - True

