# Assessment of instrument biases: ozone in the upper troposphere – lower stratosphere

**Paul S. Jeffery** (paul.jeffery@mail.utoronto.ca)[1], Kaley A. Walker[1], James R. Drummond[1,2], Luis F. Millán[3], Peter Hoor[4], Michaela I. Hegglin[5,6,7], Gloria L. Manney[8,9], Harald Boenisch[10], Daniel Kunkel[4], Irina Petropavlovskikh[11], Hao Ye[6], Thierry Leblanc[3], and Franziska M. Weyland[4]

[1]University of Toronto, [2]Dalhousie University, [3]Jet Propulsion Laboratory, [4]University of Mainz, [5]Forschungszentrum Jülich, ICE-4, [6]University of Reading, [7]University of Wuppertal, [8]NorthWest Research Associates, [9]New Mexico Institute of Mining and Technology, [10]Karlsurhe Institute of Technology, [11]National Oceanic and Atmospheric Administration

## Motivation and Focus

The Upper Troposphere – Lower Stratosphere (UTLS) region is a chemically and dynamically active part of the atmosphere, characterized by large spatial and temporal variability. This variability complicates studies of trace gases, and in turn analysis of trends and key processes. While aircraft, ground-based, balloon-borne, and satellite instruments have all been used to make measurements of this region, each form of measurement has inherent biases that complicate merging these measurements for integrated analysis.

The aim of this work is to present a new method for estimating the biases between measurement datasets. The presented approach utilizes the global MERRA-2 reanalysis to serve as a transfer function between measurement datasets, maximizing the data compared and minimizing confounding impacts from sampling or measurement biases. Bias estimates are generated for the ACE-FTS and the MAESTRO satellite instruments, both aboard the Canadian SCISAT satellite. These estimates are generated using this novel transfer function method, as well as using a typical climatology-based bias estimation method to validate the former. Focus within this work is specifically on ozone measurement biases in the UTLS.

This work is done in part to support the Atmospheric Processes And their Role in Climate (APARC) Observed Composition Trends And Variability in the Upper Troposphere and Lower Stratosphere (OCTAV-UTLS) activity.

## SCISAT

The Atmospheric Chemistry Experiment (ACE) mission, aboard the Canadian satellite SCISAT, was launched August 2003 into a low-Earth circular orbit (650 km altitude, 74° inclination)[1]. Aboard SCISAT are two solar occultation instruments, ACE-FTS and MAESTRO, which operate in a limb-viewing geometry.

ACE-FTS and MAESTRO share a single suntracker, and thus the same line-of-sight, and make measurements twice per orbit, with up to 15 sunrises and 15 sunsets measurements per day. The latitudinal coverage of the ACE instruments spans from 85°N to 85°S, with a higher measurement density in the polar regions. However, due to the inclination of SCISAT's orbit, approximately three months of measurements are required to achieve global coverage.

## ACE-FTS

**Full name**: Atmospheric Chemistry Experiment Fourier Transform Spectrometer.
**Operations**: February 2004 to present.
**Instrument Details**: An IR Fourier transform spectrometer, measuring spectra between 750 – 4400 $cm^{-1}$ with 0.02 $cm^{-1}$ spectral resolution[1].
**Measurement resolution**: Measurements are made with vertical spacing between 1.5 and 6 km and a vertical field of view (FOV) of 3 to 4 km on the limb, resulting in an effective vertical resolution of 3-4 km.
**Products**: Vertical profiles of temperature, pressure and volume mixing ratio for 11 key tracer species, 21 halogen containing species, 14 carbon containing species, and various isotopologues[2].
**Versions Used**: v5.3.
**Additional notes:** Quality flags, described in Sheese *et al.* (2015), are used to remove outliers from the dataset[3].

## MAESTRO

**Full name**: Measurement of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation.
**Operations**: February 2004 to present.
**Instrument details**: A dual UV-visible spectrometer, measuring spectra between 285 – 1030 nm with wavelength dependent resolution of 1 – 2 nm[4].
**Measurement resolution**: The 1.2 km vertical FOV on the limb coupled with measurement spacing of 1 to 2 km leads to an effective vertical resolution of 1-2 km.
**Products**: Vertical profiles of $O_3$, aerosols, optical depth, $NO_2$, and $H_2O$ (not in v4)[5,6].
**Versions Used**: v4.5/4.5b.
**Additional Notes:** Since early in the mission an unknown containment has affected the ability to retrieve trace gas profiles from the UV channel. As a result, the UV ozone and $NO_2$ products are only viable until December 2009 and June 2009, respectively[6].

## MERRA-2 and JETPAC

The Modern-Era Retrospective analysis for Research and Applications Version 2 is a global atmospheric reanalysis designed to provide ongoing near-real-time climate analysis. Reanalysis fields are provided at 0.5° x 0.625° resolution with 72 vertical levels spanning from the surface to 0.01 hPa[7]. MERRA-2 products have a vertical resolution of approximately 1.2 km in the UTLS[8-10]. The ozone gradient around the tropopause and the interannual and weekly variations in ozone are well represented.

The JEt and Tropopause Products for Analysis and Characterization (JETPAC) software package identifies and characterizes atmospheric features and fields from reanalysis datasets[9,11-13]. Of particular relevance to this study is the JETPAC algorithm's capability to calculate potential temperature and equivalent latitude, the coordinate systems used in this work. These fields are derived from MERRA-2 for the period from February 2004 to December 2020 and interpolated to the times and locations of each measurement in the datasets employed.

## Bias estimation methodologies

### Profile-to-profile comparisons

- The choice of coincidence criteria can minimize the effects of sampling biases.
- Direct profile-to-profile comparisons limit the amount of data compared to a fraction of the overall datasets.
- Comparisons might not be representative of the whole atmosphere.

### Climatological comparisons

- Emphasises the spatial distribution of the biases.
- Allows for a greater percentage of data to be used, representing more of the atmosphere.
- Sampling is not always accounted for, which can affect the comparisons.

## Transfer function methodology

Rather than these traditional approaches, this novel technique employs a reanalysis/model as a "transfer function" to allow for indirect comparisons between measurement datasets. Furthermore, subsampling the reanalysis/model and comparing it to the full reanalysis/model allows the sampling to be assessed.

Defining a measurement as the sum of three components:

$$\textit{Measurement} \approx \textit{Truth (T)} + \textit{Sampling Bias } (S_{inst}) + \textit{Measurement Bias } (B_{inst}) \quad (1)$$

We can also define a global and subsampled reanalysis as:

$$\textit{Global Reanalysis} \approx \textit{Truth (T)} + \textit{Modelling Bias } (B_{mod}) \quad (2)$$

$$\textit{Subsampled Reanalysis} \approx \textit{Truth (T)} + \textit{Sampling Bias } (S_{inst}) + \textit{Modelling Bias } (B_{mod}) \quad (3)$$

Comparing measurements (1) to subsampled reanalysis (3) leaves the relative bias:

$$(T + S_{inst} + B_{inst}) - (T + S_{inst} + B_{mod}) = (B_{inst} - B_{mod}) \quad (4)$$

For a pair of instruments (labeled 1 and 2), we can exploit the fact that within the same reanalysis, $B_{mod}$ should be consistent, yielding:

$$(B_{inst} - B_{mod})_1 - (B_{inst} - B_{mod})_2 = (B_{inst})_1 - (B_{inst})_2 \approx \text{Measurement biases} \quad (5)$$

Similarly, comparing the subsampled reanalysis (3) to the full reanalysis (2 yields:

$$(T + S_{inst} + B_{mod}) - (T + B_{mod}) = S_{inst} \quad (6)$$

And for a pair of instruments, this yields:

$$(S_{inst})_1 - (S_{inst})_2 \approx \text{Effective sampling biases} \quad (7)$$

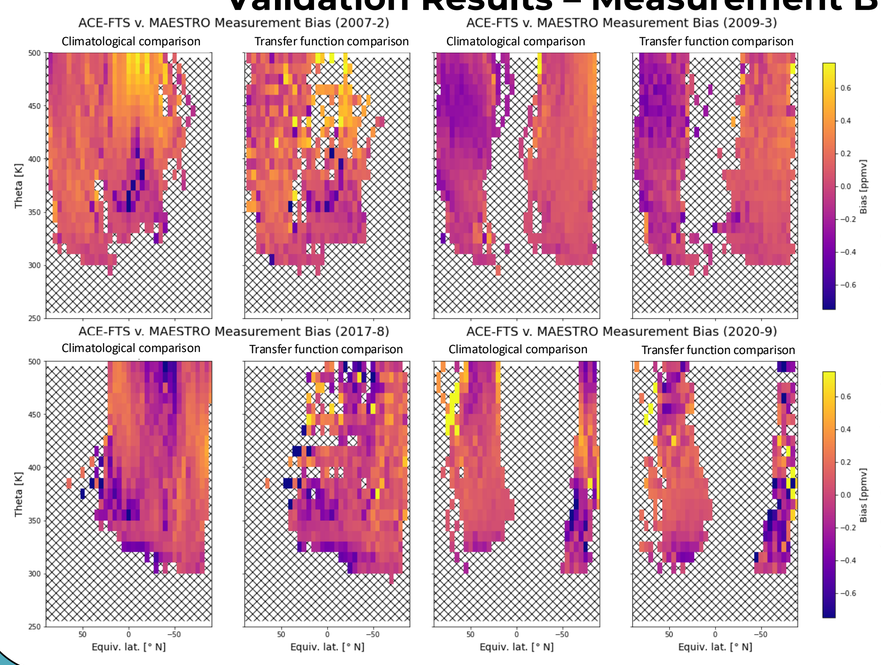
## Validation

ACE-FTS and MAESTRO share a line-of-sight and make measurements simultaneously. All MAESTRO retrievals require coincident retrieved ACE-FTS pressure and temperature information, ensuring that each measurement from MAESTRO is always coincident with a measurement from ACE-FTS. Therefore:

- Subsampling these two datasets to only measurements with a coincident successful measurement allows the measurement bias between ACE-FTS and MAESTRO to be estimated without the effect of sampling bias.
- Comparing the subsampled ACE-FTS dataset to the full ACE-FTS dataset, allows the sampling bias between ACE-FTS and MAESTRO to be estimated without the effect of measurement bias.

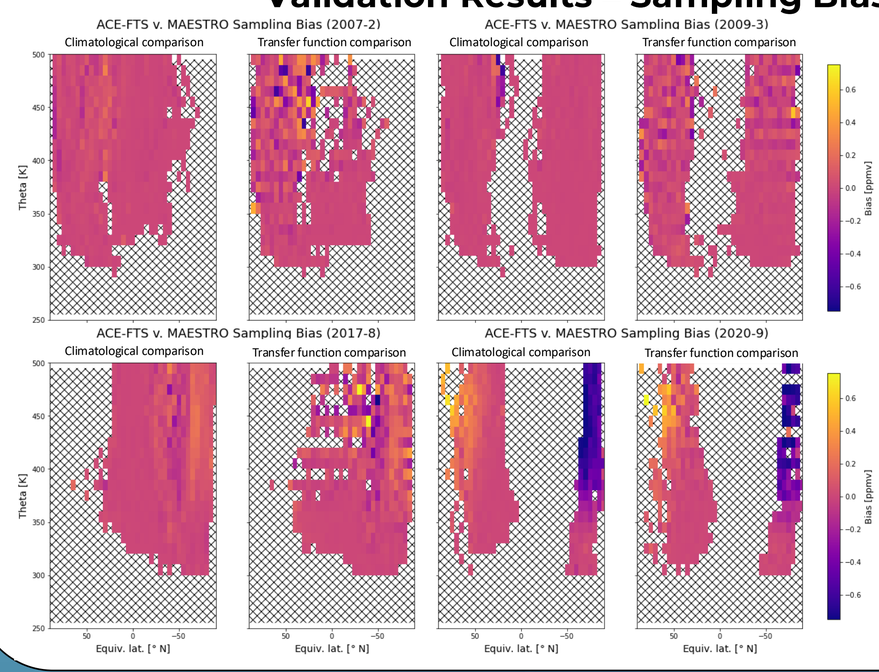
This allows for a direct approach to validating the transfer function bias estimation method.

## Validation Results – Measurement Bias



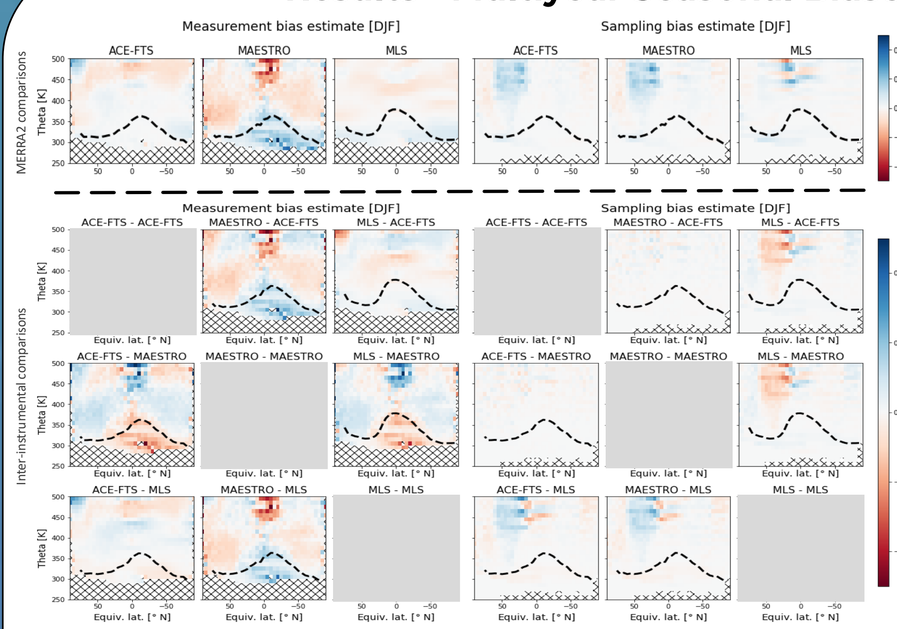

Monthly estimates of the measurement bias generated using the climatological approach (left panel of each pair) and the outlined transfer function method (right panel of each pair). Results are shown for a random selection of months. The bias estimates are found to be generally consistent with each other, illustrating the viability of this new technique.

## Validation Results – Sampling Bias




The sampling bias estimates generated using the outlined approaches are also found to be generally consistent, albeit with the appearance of an oscillating pattern of high and low biases in those produced using the transfer function approach. This pattern is likely a result of interpolation across the vertical coordinate system; however, the new technique is still found to be viable.

## Results - Multiyear Seasonal Biases




Having shown the viability of the transfer function method, here it is used to estimate the measurement (left three columns) and sampling (right three columns) biases between ACE-FTS, MAESTRO, and the Aura-MLS[14] ozone measurements in the UTLS. The top row shows the estimates in relation to MERRA-2, while the bottom three rows show the estimates between instrument pairs.

From the measurement bias estimates, it is found that ACE-FTS and Aura-MLS have the best agreement of the three instruments, with ozone biases typically within 0.1 ppmv. Larger biases are found between MAESTRO and the other instruments, particularly in the tropical lower stratosphere. Notably, the measurement bias tends to follow the tropopause, with differing measurement biases above and below. For the sampling biases, ACE-FTS and MAESTRO show little difference, as expected given their shared line-of-sight. The relative sampling bias with Aura-MLS and the SCISAT instruments is a result of their different observational coverage.

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