TES Data for Assimilation, Inverse modeling and intercomparison

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Kevin W. Bowman, D.B. Jones[1], J. Worden, Q. Li, S. Sund-Kulawik, H. Worden, G. Osterman, A. Eldering, M. Luo, M. Lampel[2], D. Jacob[3], D. Rider, B. Fisher

Jet Propulsion Laboratory-Cal Tech, [1]University of Toronto, [2]Raytheon Systems-ITSS, [3]Harvard University

ABSTRACT

The TES retrieval algorithm estimates an atmospheric profile by simultaneously minimizing the difference between observed and model spectral radiances subject to the constraint that the solution is consistent with an a priori mean and covariance. Consequently, the retrieved profile includes contributions from observations with random and systematic errors and from the prior. These contributions must be properly characterized in order to use TES retrievals in data assimilation, inverse modeling, averaging, and intercomparison with other measurements. All TES retrievals include measurement and systematic error covariances along with averaging kernel and a priori vector. We illustrate how to use these TES data with a couple of examples from a simulated CO source estimation and comparison of TES ozone retrieval to the GEOS-CHEM chemical transport model.

Characterization of TES retrievals

If the estimate of a profile is spectrally linear with respect to the true state then the retrieval may be written as

$$\hat{\mathbf{y}}_t^i = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\mathbf{y}_t^i - \mathbf{y}_{t,c}^i) + \varepsilon_t^i$$

$\hat{\mathbf{y}}_t^i$: vertical trace gas profile at time t and location i

$\mathbf{y}_{t,c}^i$: constraint profile

$\mathbf{y}_t^i$: true state of trace gas profile

$\mathbf{A}_t^i$: averaging kernel

There are 3 errors included in the analysis: $\varepsilon_t^i = \varepsilon_n^i + \varepsilon_{cs}^i + \varepsilon_b^i$

Measurement noise: $\varepsilon_n^i = \mathbf{G}^i\mathbf{n}^i$

Cross-state error: $\varepsilon_{cs}^i = \sum_l \mathbf{A}_l^{cs}(\mathbf{s}^i - \mathbf{s}_c)$

Systematic error from non-retrieved species Spectroscopy, etc.: $\varepsilon_s^i = \sum_l \mathbf{G}^i\mathbf{K}_l^i(\mathbf{b}_l^i - \mathbf{b}_{l,c}^i)$

A retrieval characterized by the averaging kernel and constraint vector can be used to quantitatively compare model fields directly TES vertical profiles:

If the model fields are defined as

$\mathbf{y}_t^{i,m} = \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t)$ where

$\mathbf{x}$: model fields

$\mathbf{u}$: model parameters, e.g, sources and sinks

$\mathbf{F}$: model operator, range is vmr for trace gases

Then the model TES retrieval for trace gases is

$$\hat{\mathbf{y}}_t^{i,m} = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\ln \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t) - \mathbf{y}_{t,c}^i)$$

The *observation operator* can be written as

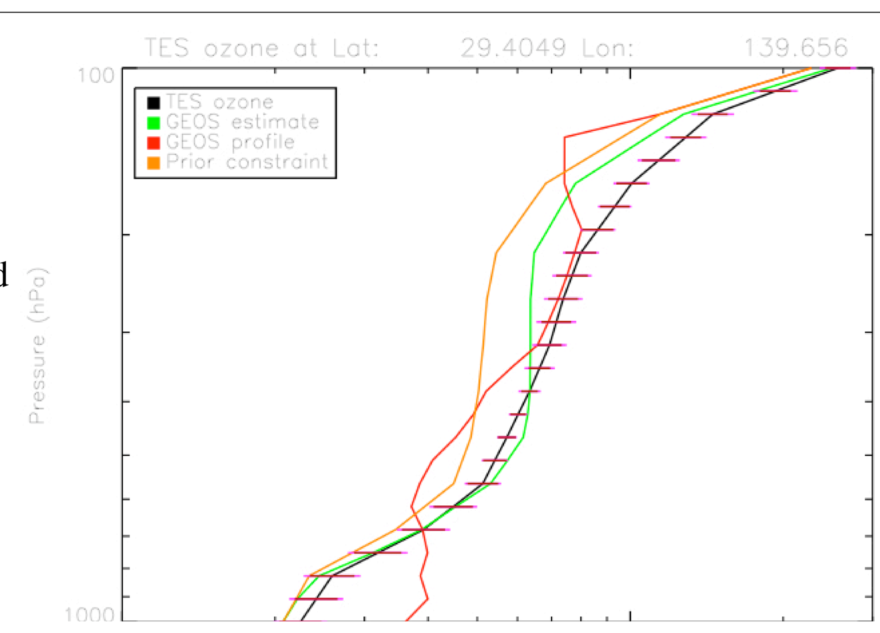
$$\mathbf{H}_t(\mathbf{x}_t, \mathbf{u}_t, t) = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\ln \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t) - \mathbf{y}_{t,c}^i)$$

From the standpoint of the model, the observations are now expressed in the standard additive noise model

$$\hat{\mathbf{y}}_t^i = \mathbf{H}(\mathbf{x}_t, \mathbf{u}_t, t) + \varepsilon$$

This TES ozone retrieval was taken From an observation near the island of Sumisu-jima off the coast of Japan on Sept 20, 2004. The green profile was calculated by substituting The natural logarithm of a GEOS-CHEM model field (2x2.5 degrees) was substituted into the model TES retrieval equation.

Both the GEOS-CHEM model and the TES retrieval indicate elements amounts of ozone in the upper troposphere, consistent with Asian pollution outflow into the Pacific. However, the TES retrieval suggests a greater amount of ozon relative to GEOS-CHEM. Understanding the differences between the two requires additional statistics within the grid.

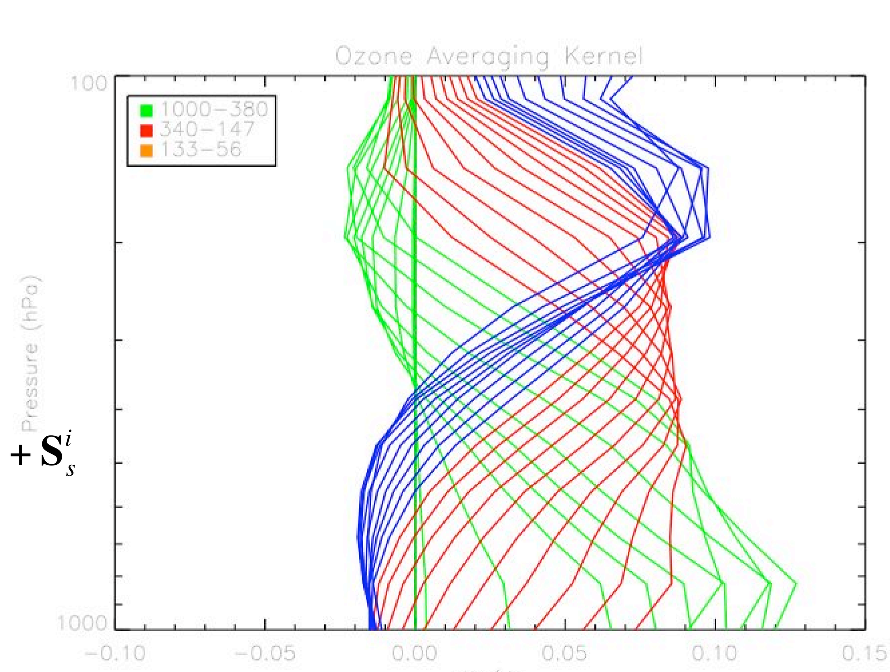


The error covariance for the difference between model retrieval and the TES retrieval is

$$\hat{\mathbf{S}} = \mathbf{A}_t^i(E[((\mathbf{y}_t^i - \ln \mathbf{F}) - \overline{\mathbf{y}_t^i - \ln \mathbf{F}})^2]\left(\mathbf{A}_t^i\right)^{\mathrm{T}} + \mathbf{S}_n^i + \mathbf{S}_{cs}^i + \mathbf{S}_s^i$$

Supplied by user

Supplied by TES L2 processing



Mapping (interpolation) and the averaging kernel

The averaging kernel is the sensitivity of the Retrieved profile to changes in the true state and Is composed of 3 matrices:

$$\mathbf{A}_t^i = \frac{\partial \hat{\mathbf{y}}_t^i}{\partial \mathbf{y}_t^i} = \mathbf{M}^i\mathbf{G}_z^i\mathbf{K}_y^i$$

Mapping (interpolation) matrix:

$$\mathbf{y}_t^i = \mathbf{M}\mathbf{z}_t^i, \qquad \mathbf{M} : {}^{\circ\, M} \to {}^{\circ\, N}, \; M < N$$

The mapping matrix projects the retrieval coefficients to the forward model levels. This mapping represents a "hard" constraint on the estimated profile, .i.e, restricts the profile to a subspace defined by **M**.

The averaging kernel is supplied on the forward model Pressure grid, which is nominally 87 levels where each level Is approximately 1.5 km. The degrees of freedom for signal Dofs for any TES retrieval is significantly less than 87. So, why Do we store them on such a fine scale?

Gain matrix:

$$\mathbf{G}_z^i = \left(\left(\mathbf{K}_y\mathbf{M}\right)^{\mathrm{T}} \mathbf{S}_n^{-1}\mathbf{K}_y\mathbf{M} + \Lambda\right)^{-1}\left(\mathbf{K}_y\mathbf{M}\right)^{\mathrm{T}}\mathbf{S}_n^{-1}$$

The gain matrix projects the TES observed radiances o the TES estimate profiles based on the TES spectral Jacobian, hard constraints, and prior or "soft" constraint Λ.

Spectral Jacobian matrix: $\mathbf{K}_y = \dfrac{\partial \mathbf{L}}{\partial \mathbf{y}}$

- •Averaging kernel on a fine pressure scale accommodates a variety grids, e.g., balloons, tropospheric models, stratospheric models, column trace gas observations
- •Averaging kernel can be reduced without loss of information but not vice versa
- •Subsequent changes in the retrieval, e.g., changes in **M**, do not change file format.

Examples of mapping:

$\mathbf{M}_{Trop} : {}^{\circ\, P} \to {}^{\circ\, N}$ Tropospheric CTM, most levels in troposphere. few in stratosphere.

$$\hat{\mathbf{y}}_t^{i,m} = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\mathbf{M}_{Trop} \ln \mathbf{F}(\cdot) - \mathbf{y}_{t,c}^i)$$

$\mathbf{M}_c : {}^{\circ} \to {}^{\circ\, N}$ Fixed profile mapping

$\mathbf{h}^{\mathrm{T}} : {}^{\circ\, N} \to {}^{\circ}$ Column operator

$$\hat{c}_t^i = \mathbf{h}^T\hat{\mathbf{y}}_t^i = \mathbf{h}^T\mathbf{y}_{t,c}^i + \mathbf{h}^T\mathbf{A}_t^i(\ln(\mathbf{M}_c\alpha) - \mathbf{y}_{t,c}^i)$$

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Assimilation of TES data for use in model parameter and field estimation

Characterization of TES retrievals is critical for applications where TES data is assimilated into a model such as model parameter and field estimation. This approach several advantages:
•The relationship between the true state and estimated profile is *linear*. The nonlinearity between the prior and the true state has been removed
•The effects of the mapping, constraint matrix and vector, and spectral sensitivity have been incorporated in the characterization.
•Tens of thousands of spectral channels have been reduced to a much smaller geophysical parameter set.

Application to model parameter estimation: CO source estimation

We investigate the impact of the averaging kernel on model CO source estimation with simulated TES retrievals. In the CO estimation problem, The model CO sources are parameterized according to a geographical Aggregation as shown in Figure 1. Simulated TES retrievals are used to Estimate these CO source strengths relative to a background or prior Knowledge of those strengths. This estimate is calculated by minimizing The following cost functions with and without the averaging kernel:

$$C_{AK}(\mathbf{u}) = \left\|\hat{\mathbf{y}} - \mathbf{H}(\mathbf{x},\mathbf{u},t)\right\|^2_{\mathbf{S}_\varepsilon^{-1}} + \left\|\mathbf{u} - \mathbf{u}_a\right\|^2_{\mathbf{S}_a^{-1}}$$

$$C_{woAK}(\mathbf{u}) = \left\|\hat{\mathbf{y}} - \ln\mathbf{F}(\mathbf{x},\mathbf{u},t)\right\|^2_{\mathbf{S}_\varepsilon^{-1}} + \left\|\mathbf{u} - \mathbf{u}_a\right\|^2_{\mathbf{S}_a^{-1}}$$

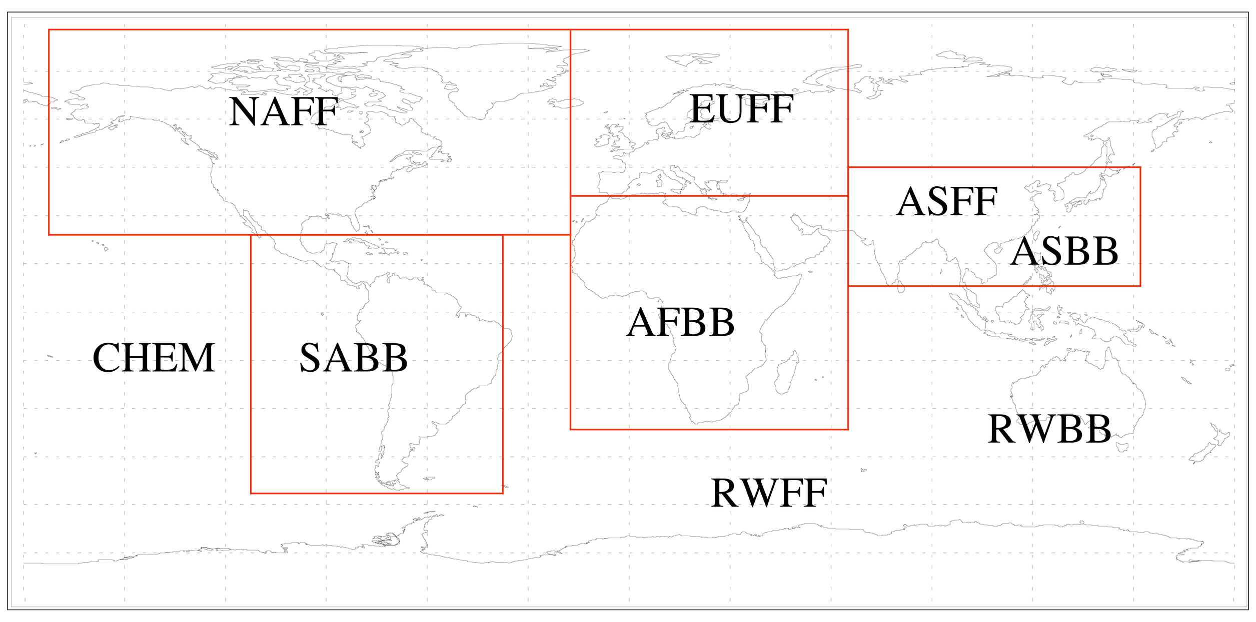

Figure 1: CO source aggregation. Taken from Jones, D. B. A., K. W. Bowman, P. I. Palmer, J. R. Worden, D. J. Jacob, R. N. Hoffman, I. Bey, and R. M. Yantosca, Potential of observations from the Tropospheric Emission Spectrometer to constrain continental sources of carbon monoxide, J. Geophys. Res., 108(D24), 4789, doi:10.1029/2003JD003702, 2003.

- FF = Fossil Fuel + Biofuel
- All sources include contributions from oxidation of VOCs
- OH is specified
- Use a "tagged CO" method to estimate contribution from each source
- Temporal evolution of emissions is known.

CO source state vector:
•CHEM-background chemistry
•NAFF-North American fossil fuel
•EUFF-European fossil fuel
•AFBB-African biomass burning
•ASFF-Asian fossil fuel
•ASBB-Asian biomass burning
•RWBB-rest-of-the-world biomass burning
•RWFF-rest-of-the-world fossil fuel
•SABB-South American biomass burning

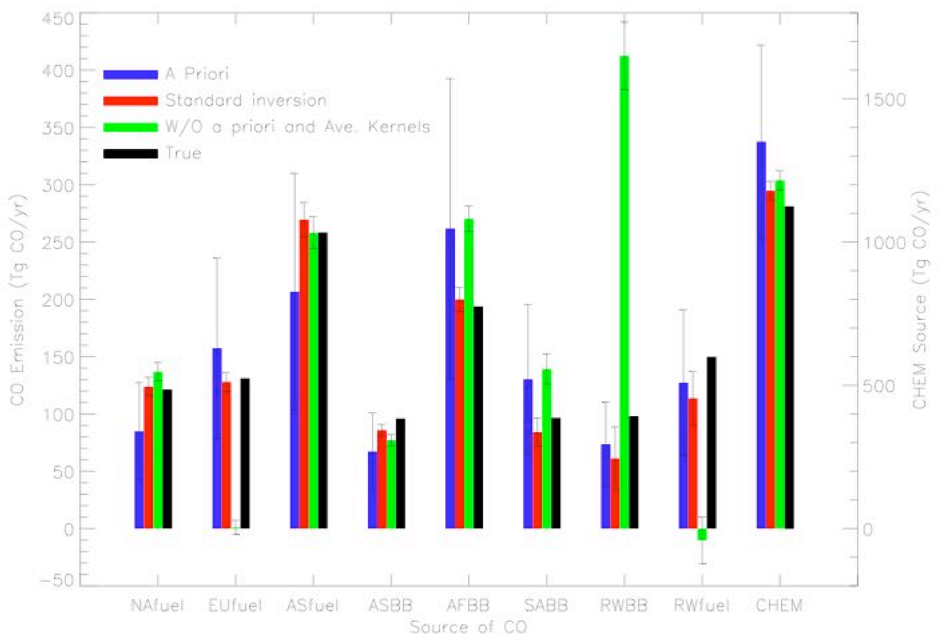

Figure 2: Estimate of CO aggregated sources with And without the averaging kernels.

Neglecting the averaging kernels has two effects on the CO source estimate:

1. The CO source estimates are grossly inaccurate
2. The number of iterations to convergence increased by a factor of 2 with increase numerical instability.

On the other hand, proper use of the averaging kernel shows The potential of TES CO retrievals to constrain estimates of Continental source of carbon monoxide.

Conclusions

•TES Level 2 products will include, along with retrievals of atmospheric trace gases, averaging kernels, constraint vectors, and error covariance matrices on the forward model levels
•These tools can be used profitably by atmospheric sciences community for comparison of TES retrievals to *in-situ* sonde measurements, aircraft and satellite measurements, along with comparison to chemical transport models.
•These techniques enable assimilation systems to properly incorporate TES data by characterizing the constraints and biases used in the retrieval without resorting to expensive and non-linear radiative transfer models

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