Tropospheric CO Observed with NAST-I: Retrieval Algorithm, First Results, and Validation

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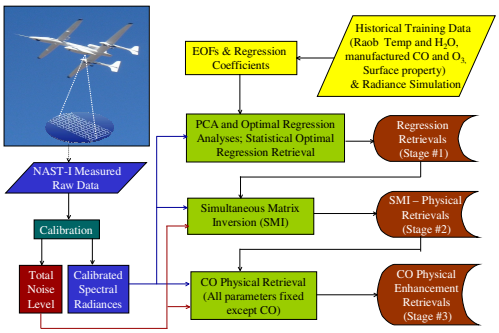
ABSTRACT. A methodology of retrieving tropospheric carbon monoxide (CO) from remotely sensed infrared (IR) spectral data has been developed. Tropospheric CO profiles, together with thermodynamic properties, are determined using a three-stage approach that combines the algorithms of physical-based statistical eigenvector regression, simultaneous non-linear radiance inversion, and CO enhanced physical iterative retrieval. The NPOESS Airborne Sounder Testbed-Interferometer (NAST-I) aboard a high altitude aircraft with a spectral coverage of 650-2700 cm^{-1} and a spectral resolution of 0.25 cm^{-1} has been successfully collecting data throughout many field campaigns. The retrieval methodology is described and demonstrated by simulations. Detailed CO retrieval error analyses based on the NAST-I instrument and retrieval uncertainties of the other parameters are discussed. Results from several NAST-I field campaigns are presented including those from observations over the western Pacific Ocean made in conjunction with airborne truth atmospheric chemistry profiles. Retrievals from both simulations and measurements illustrate that tropospheric CO profiles can be obtained from remotely sensed IR spectral data (such as NAST-I data) with accurate thermodynamic properties.

1. Flow Diagram for NAST-I Data



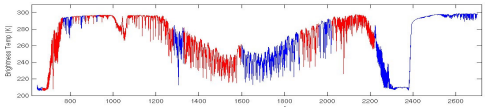
2. NAST-I Regression Inversion Methodology

$$M_{ij} = \frac{1}{S}\sum_{k=1}^{S} \Re_{ki}\,\Re_{kj}$$

$$C_i = \sum_{j=1}^{nc} \Re_j\, U_{ji}$$

$$A_j = \sum_{i=1}^{n-1} K_{ji}\, C_i + K_{jn} P_s = \sum_{i=1}^{n-1} K_{ji} \left(\sum_{l=1}^{nc} \Re_l U_{li}\right) + K_{jn} P_s$$

R = radiance
$\Re$ = radiance deviation from the mean
ε = surface emissivity
P_s = surface pressure
S = number of sample profiles
M = covariance matrix of $\Re$
U = eigenvectors of M
C = radiance EOF amplitudes
A = {T_s, ε, T, q, o3, co, …} parameters
K = regression coefficient



The spectral regions indicated in red are used in the regression retrieval.

3. NAST-I Simultaneous Matrix Inversion

$$Y = \varepsilon B_s \tau_s - \int_{P_{ac}}^{P_s} B\,d\tau + (1-\varepsilon)\int_{P_{ac}}^{P_s} B\,d\tau^*, \quad \tau^* = \tau_s^2/\tau$$

$$\delta Y = Y'\,\delta X$$

$$J(X) = [Y^m - Y(X)]^T E^{-1} [Y^m - Y(X)] + [X - X_0]^T (\gamma I)[X - X_0]$$

$$X_{n+1} = X_n + J^*(X_n)^{-1} J'(X_n)$$

$$\delta X_{n+1} = (Y_n'^T E^{-1} Y_n' + \gamma I)^{-1} Y_n'^T E^{-1} (\delta Y_n + Y_n' \delta X_n)$$

$$\delta X_n = X_n - X_0, \quad \delta Y_n = Y^m - Y(X_n)$$

$$\left\| Y[X(\gamma)] - Y^m \right\|^2 = \sigma^2, \quad \gamma_{n+1} = q_n \gamma_n$$

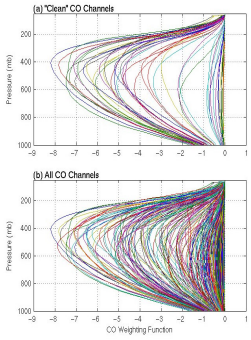
q is a factor for increasing or decreasing, which is obtained in each iteration by satisfying the following conditions or the maximum iteration reaches 10.

$$q_n = 1.0;$$
$$\text{if } \left\|Y(X_n) - Y^m\right\| < \sigma^2, \text{ then } q_n = 1.5;$$
$$\text{if } \left\|Y(X_n) - Y^m\right\| = \sigma^2, \text{ then stop the iteration;}$$
$$\text{if } \left\|Y(X_n) - Y^m\right\| > \sigma^2, \text{ then } q_n = 0.5;$$

Simultaneous matrix inversion retrieval (using minimum discrepancy principle)

Y = cal. Radiance
ε = surface emissivity
τ = transmittance
B = Planck radiance
P = pressure
s = surface
X = {T_s, ε, T, q, o3, co}
Y^m = obs. Radiance
J = "Penalty function"
σ = total noise
T denotes the transpose
E = error covariance matrix
γ = a smoothing factor
n = iteration number

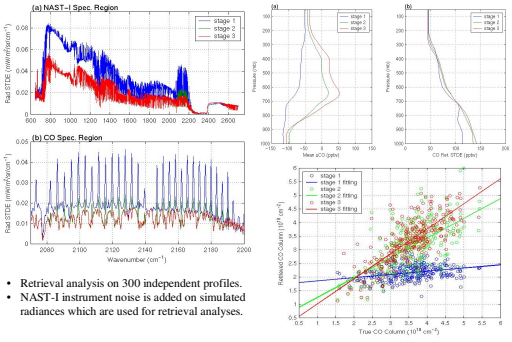
4. CO Physical Enhancement Iteration



- All CO sensitive channels can be used.
- Retrieval channels are limited to CO sensitive channels.
- All parameters, except the CO profile, are fixed in the iteration (use the retrieval from retrieval stage 2). The state vector $X_n = X_0\{T_s, \varepsilon, T, q, o3\} + X_1\{co\}$, where X_0 is a constant vector in this stage.
- Physical retrieval is repeated for CO profile enhancement retrieval, using the iteration criteria for achieving best CO retrieval accuracy in each iteration by satisfying the following conditions or the maximum iteration reaches 4.

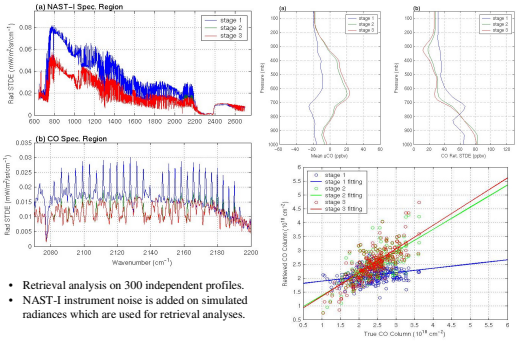
$$q_n = 1.0;$$
$$\text{if } \left\|Y(X_n) - Y^m\right\| < \sigma^2, \text{ then } q_n = 1.2;$$
$$\text{if } \left\|Y(X_n) - Y^m\right\| = \sigma^2, \text{ then stop the iteration;}$$
$$\text{if } \left\|Y(X_n) - Y^m\right\| > \sigma^2, \text{ then } q_n = 0.8;$$

5. CO Retrieval Simulation (50% enlarged CO)



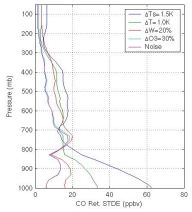
- Retrieval analysis on 300 independent profiles.
- NAST-I instrument noise is added on simulated radiances which are used for retrieval analyses.

6. CO Retrieval Simulation (nominal CO)



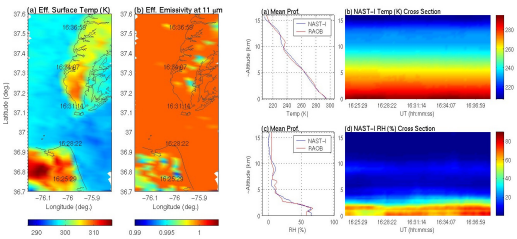
- Retrieval analysis on 300 independent profiles.
- NAST-I instrument noise is added on simulated radiances which are used for retrieval analyses.

7. CO Retrieval Error Simulation



- Retrieval analysis on 300 independent profiles.
- NAST-I instrument noise is added on simulated radiances which are used for retrieval analyses.
- Assume that the vertical weighting uncertainty through the CO retrieval processing is ignored; and the first guess CO profile is the truth.
- CO enhancement retrieval is performed with the true parameters as the first guesses, except one of them is perturbed.
- The retrieved CO profiles are then compared with the truth to compute the STDE contributed by that perturbed parameter.
- Other errors introduced by the sources such as CO line intensity uncertainty should also be considered.
- An error can also be introduced by the first guess due to poor vertical resolution and sensitivity distribution (shown above).

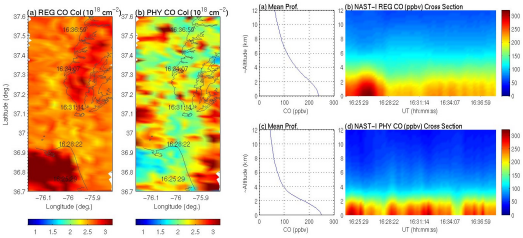
8. NAST-I Retrieval Sample (July 14, 2001)



Retrieved surface properties from NAST-I flight. The UT associated with geophysical location is indicated in the figure.

NAST-I temperature and moisture profile cross-section of the simultaneous matrix inversion and their mean profiles of the cross-sections in comparison with a nearby radiosonde.

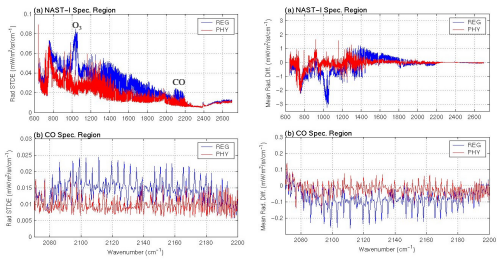
9. NAST-I Retrieval Sample (July 14, 2001)



NAST-I CO column densities of (a) regression as first guesses (with a mean of 2.7×10^{18} cm^{-2}) for (b) physical retrievals (with a mean of 2.2×10^{18} cm^{-2}).

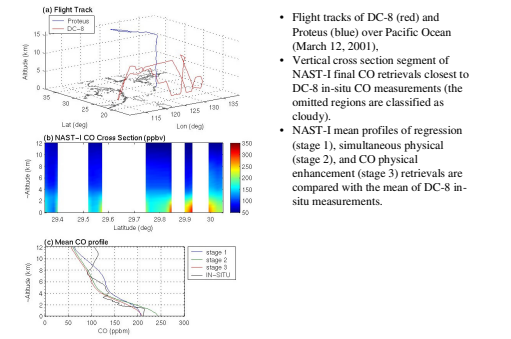
NAST-I CO profile cross-section of regression as first guesses, and physical enhancement retrieval, and their mean profiles of the cross-sections.

10. Retrieval Validation – Radiance (July 14, 2001)



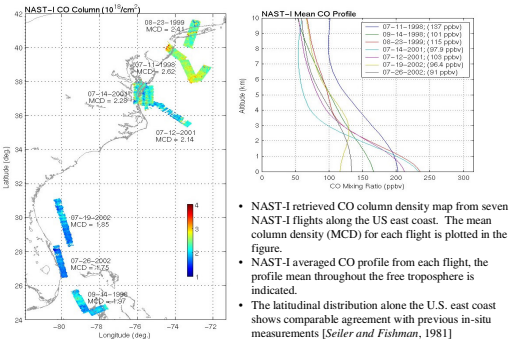
- The statistical analyses of STDE and the mean difference between observed and retrieval-calculated radiances over the retrieved samples (a total of 910 samples).
- Radiance convergence is achieved, shown in both the STD error as well as the mean difference, especially in the spectral regions of trace species (i.e., H_2O, O_3, CO).

11. Retrieval Validation - Profile (March 12, 2001)



- Flight tracks of DC-8 (red) and Proteus (blue) over Pacific Ocean (March 12, 2001),
- Vertical cross section segment of NAST-I final CO retrievals closest to DC-8 in-situ CO measurements (the omitted regions are classified as cloudy).
- NAST-I mean profiles of regression (stage 1), simultaneous physical (stage 2), and CO physical enhancement (stage 3) retrievals are compared with the mean of DC-8 in-situ measurements.

12. CO Summer Column Density on US East Coast



- NAST-I retrieved CO column density map from seven NAST-I flights along the US east coast. The mean column density (MCD) for each flight is plotted in the figure.
- NAST-I averaged CO profile from each flight, the profile mean throughout the free troposphere is indicated.
- The latitudinal distribution alone the U.S. east coast shows comparable agreement with previous in-situ measurements [*Seiler and Fishman*, 1981]

SUMMARY. An inversion algorithm for tropospheric CO profile retrieval from FTS nadir observation has been developed, tested, and demonstrated using NAST-I measurements. In particular, the CO profile retrieval approach is developed and analyzed using forward and inverted simulations together with NAST-I measurements for retrieval tests. This verifies the integrity of this retrieval application. NAST-I CO retrieval samples demonstrate the ability of this retrieval algorithm not only to capture temperature and moisture profile variations but CO variations as well. Furthermore, the vertical profile comparison with nearby in-situ measurements of March 12, 2001 shows a reasonable agreement. These preliminary results demonstrate that the CO profiles are retrieved from accurate nadir-observations of high-spectrally resolved radiances as can be achieved with an FTS. Additional validation analyses are desired in order to provide more definitive conclusions.

References:
- W. L. Smith et al., "NAST-I: results from revolutionary aircraft sounding spectrometer", in *SPIE Proceedings* **3756**, 2–8 (1999).
- D. K. Zhou et al., "Thermodynamic product retrieval methodology for NAST-I and validation," *Applied Optics*, **41**, 6,957–6,967 (2002).
- W. Seiler, and J. Fishman, "The distribution of carbon monoxide and ozone in the free troposphere," *J. Geophys. Res.*, **86**, 7,225–7,265 (1981).