

Retrieval of Tropospheric Carbon Monoxide Profiles from MOPITT: Algorithm Description and Retrieval Simulation

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ABSTRACT

The Measurement of Pollution in the Troposphere (MOPITT) instrument is an eight-channel gas correlation radiometer to be launched on the Earth Observing System (EOS) Terra spacecraft in 1999. Its main measurement objectives are tropospheric carbon monoxide (CO) profiles and total column. This paper gives a detailed description of MOPITT CO retrieval algorithm, which derives total CO column and tropospheric CO mixing ratios at a number of atmospheric pressure levels from MOPITT radiance observations. Retrieval performance evaluation using simulated MOPITT data are discussed.

Keywords: MOPITT, carbon monoxide, retrieval, tropospheric chemistry

1. INTRODUCTION

There have been increasing worldwide concerns and awareness of possible human impact on the environment and climate change. To address these concerns and gain a better understanding of the connection between increased human activities and global climate change, sophisticated satellite-borne remote sensors are being developed to measure the global distribution of trace gases that are important in the study of global air pollution and global tropospheric chemistry. Some of the important trace gases to be measured by satellite instruments in the next decade or so include H₂O, O₃, CO, CH₄, etc. A better understanding of the global distributions, trends, variability, sources and sinks of these gases will advance our knowledge of the relationships between human activities and the natural environment.

CO is one of the important trace gases in tropospheric chemistry. Its concentration in the troposphere directly affects the concentration of tropospheric hydroxyl (OH), which regulates the lifetimes of many tropospheric trace gases.¹ CO can also be used as a tracer to study the transport of global and regional pollutants from industrial activities and large-scale biomass burning. Many research groups around the world have been conducting surface and tropospheric CO measurements using ground-based and airborne instruments. There is a global surface CO monitoring network, the Climate Monitoring and Diagnostic Laboratory of the National Oceanic and Atmospheric Administration (NOAA/CMDL) Cooperative Air Sampling Network (<http://www.cmdl.noaa.gov/ccg/flask/sites.html>). It includes 4 NOAA/CMDL baseline observatories, 40 cooperative sites, 4 commercial vessels, and 2 sites located on towers. Gas species measured are CO₂, CH₄, CO, N₂O, SF₆, and the carbon and oxygen isotopes of CO₂. To our knowledge, there are only two sites around the world where tropospheric CO profiles are measured on a routine basis using airborne sampling techniques. One site is at Carr, Colorado in the United States. It is operated by the carbon cycle group of NOAA/CMDL in Boulder, Colorado. Tropospheric CO profiles have been measured at this site on a biweekly basis using an automated airborne sampling unit since November 1992.³ The other site is located at Cape Grim in Australia. It is operated by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) of Australia. Tropospheric CO profiles have been measured on a routine basis using airborne sampling techniques since May 1992.^{4,5} Additionally, there were two shuttle missions totaling about four weeks in 1994, during which CO total column were measured by a spaceborne instrument called Measurement of Air Pollution from Space (MAPS).

Surface and boundary layer CO measurements at the NOAA/CMDL Cooperative Air Sampling Network, regular airborne CO sampling at Carr and Cape Grim, satellite observations by MAPS, and CO measurements by short duration campaigns all indicate that CO is highly variable both temporally and spatially. There are strong needs for systematic global observations by sensitive spaceborne sensors. The Measurement of Pollution In The Troposphere (MOPITT) instrument is one of the experiments selected to meet these needs. It is scheduled for launch on the Earth Observing System (EOS) Terra spacecraft in 1999. MOPITT will measure the global distribution of CO and CH₄ with a nominal horizontal resolution of 22 km by 22 km. In this paper, we will first give a brief discussion of MOPITT instrument characteristics that will facilitate

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the understanding of the MOPITT CO retrieval algorithm in section 2. Details of the algorithm for the retrieval of tropospheric CO profiles and total CO column from MOPITT observations are described in section 3. Results using simulated MOPITT data are discussed in section 4.

2. MOPITT INSTRUMENT CHARACTERISTICS

MOPITT is an eight-channel gas correlation radiometer selected for the Earth Observing System (EOS) Terra spacecraft to be launched in 1999.⁹ Its primary objectives are the measurement of tropospheric carbon monoxide (CO) profile and methane (CH₄) column. MOPITT measures upwelling thermal emission from the atmosphere and surface in the thermal channels, and reflected solar radiation in the solar channels that has passed through the atmosphere, been reflected at the surface, and transmitted back up through the atmosphere.

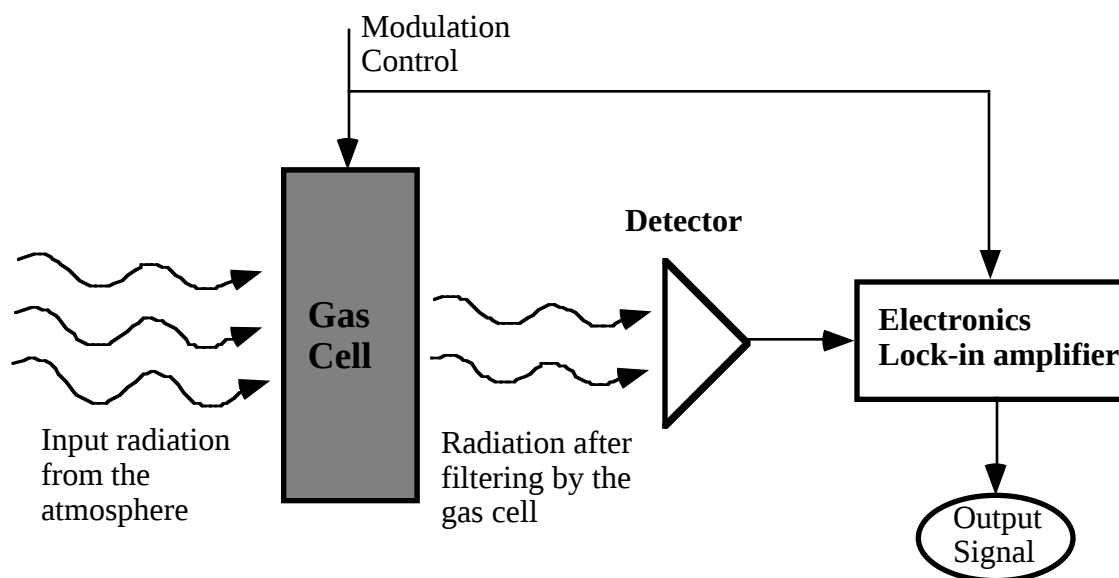


Figure 1. Schematic diagram of a gas correlation radiometer. The gas cell containing the gas of interest provides the high resolution capability.

A schematic diagram of a gas correlation radiometer is shown in figure 1. MOPITT makes use of two methods to modulate the transmittance in the gas cell. The first is by varying the cell pressure through the use of pressure modulated cells which was described in detail by Taylor (1983).¹⁰ The second is by varying the amount of gas in the cell through length modulated cells.¹¹ Two pressure modulated radiometers (PMRs) with different mean pressures and four length modulated radiometers (LMRs) are used in MOPITT. Separating the 2.3 μm and 4.7 μm channels with dichroic beam splitters results in 8 separate spectral channels. The LMR channels contain cells with higher pressure to optimize instrument sensitivity to the lower and middle troposphere, and the PMR channels contain cells with lower pressure to optimize instrument sensitivity to the upper troposphere. Each channel produces an average signal (S_A), which is the average of the instrument signals corresponding to the two states of the modulating cell, and a difference signal (S_D), which is the difference of the instrument signals corresponding to the two states of the modulating cell. Both the average signals, S_A , and the difference signals, S_D , are generated by the instrument signal processing unit (SPU) using a demodulation technique. For the LMC channels, the two states are defined by the two alternative cell path lengths of 2 mm and 10 mm. For the PMC channels, the two states are defined by the alternative high and low cell pressure. Radiative transfer calculations indicate that the difference signals are more sensitive to atmospheric CO and CH₄ changes, and the average signals are more sensitive to Earth surface and cloud characteristics. Some characteristics of the MOPITT instrument are summarized in Table 1.

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Table 1. Characteristics of MOPITT CO and CH₄ channels. There are four CO thermal channels, two CO solar channels and two CH₄ solar channels. The nominal PMC and LMC cell pressure, temperature and length are also listed.

Ch #	Primary Purpose	Modulator Type	Cell Pressure (mb)	Cell Temperature (K)	Cell Length (mm)	Center Wavenumber (1) (cm ⁻¹)
1	CO	LMC1	200	300	2 - 10	2166 (52)
2	CO	LMC1	200	300	2 - 10	4285 (40)
3	CO	PMC1	50 -100	300	10	2166 (52)
4	CH ₄	LMC2	800	300	2 - 10	4430 (140)
5	CO	LMC3	800	300	2 - 10	2166 (52)
6	CO	LMC3	800	300	2 - 10	4285 (40)
7	CO	PMC2	25 - 50	300	10	2166 (52)
8	CH ₄	LMC4	800	300	2 - 10	4430 (140)

(1) Numbers in parenthesis are band filters full width at half maximum (FWHM).

3. MOPITT CO RETRIEVAL ALGORITHM

As discussed in section 2, MOPITT has 6 CO sounding channels. The 6 CO channels generate 12 signals, 6 average signals and 6 difference signals. These are the signals to be used in a process called retrieval, in which tropospheric CO profiles and total CO column are derived. Problems of deriving geophysical parameters from radiance or transmittance measurements are often referred to as the inverse problem. As described in numerous papers and books^{12,13}, the inverse problem in remote sounding is typically ill-conditioned. There is no unique solution to the problem without additional information or constraints. Many different techniques have been developed to solve the inverse problem. One of the widely used techniques is the maximum likelihood method.¹² This technique allows the combination of current observations with prior knowledge to arrive at the most likely solution to the inverse problem in a statistical sense. Observation noises and prior knowledge uncertainties are used as weights in the form of covariance matrices. The MOPITT CO retrieval algorithm is based on the maximum likelihood method. Details of the algorithm are discussed in the following sections.

MOPITT CO thermal channel signals (channel 1, 3, 5, and 7) are calculated by equation (1) and (2). MOPITT CO solar channel signals (channel 2 and 6) are calculated by equation (3) and (4).

$$S_a^{thm} = \int_{\nu} \left\{ I_s(\nu) + \int_0^{\infty} [B(\nu, T(z)) - I_s(\nu)] \frac{d\tau(\nu, z, \infty)}{dz} dz \right\} \tau_f(\nu) \left[\frac{\tau_c(p_l) + \tau_c(p_h)}{2} \right] d\nu \quad (1)$$

$$S_d^{thm} = \int_{\nu} \left\{ I_s(\nu) + \int_0^{\infty} [B(\nu, T(z)) - I_s(\nu)] \frac{d\tau(\nu, z, \infty)}{dz} dz \right\} \tau_f(\nu) [\tau_c(p_l) - \tau_c(p_h)] d\nu \quad (2)$$

$$S_a^{sol} = \int_{\nu} R_s(\nu) I_{\Theta}(\nu) \exp \left[- \int_0^{\infty} k(z) \rho_{co}(z) (\sec(\theta_{sat}) + \sec(\theta_{Sun})) dz \right] \tau_f(\nu) \left[\frac{\tau_c(p_l) + \tau_c(p_h)}{2} \right] d\nu \quad (3)$$

$$S_d^{sol} = \int_{\nu} R_s(\nu) I_{\Theta}(\nu) \exp \left[- \int_0^{\infty} k(z) \rho_{co}(z) (\sec(\theta_{sat}) + \sec(\theta_{Sun})) dz \right] \tau_f(\nu) [\tau_c(p_l) - \tau_c(p_h)] d\nu \quad (4)$$

Where S_a^{thm} stands for CO thermal channel average signal, and S_d^{thm} stands for CO thermal channel differential signal. S_a^{sol} stands for CO solar channel average signal, and S_d^{sol} stands for CO solar channel difference signal. $I_s(\nu)$ is the top of the atmosphere radiance. $B(\nu, T(z))$ is the Planck function. $\tau(\nu, z, \infty)$ is the atmospheric transmittance from altitude z to TOA. $\tau_f(\nu)$ is the MOPITT instrument transfer function. $\tau_c(p_l)$ is the CO cell transmission function at low cell pressure of p_l . $\tau_c(p_h)$ is the CO cell transmission function at low cell pressure of p_h . $R_s(\nu)$ is the surface reflectivity in MOPITT CO solar channels. $I_o(\nu)$ is the solar irradiance at TOA. $K(z)$ is the CO absorption coefficient in CO solar channels. $\rho_{co}(z)$ is CO number density at altitude z . θ_{sat} is the MOPITT observation zenith angle. θ_{sol} is the solar zenith angle. In the MOPITT operational retrieval, these signals are calculated by a special purpose MOPITT fast radiative transfer model, called MOPFAS. Details of MOPFAS can be found at Edwards *et al.* (1999).¹⁴

The signal equations (1) to (4) can be generalized as the following equation (equation (5)), which relates the instrument signals to profiles of the target gas (CO), other interference gases profiles, Earth surface parameters, and MOPITT instrument functions.

$$Y = F(X, b) + N_{inst} \quad (5)$$

Where Y is the measurement vector consisting of 8 MOPITT CO thermal channel signals (4 average signals and 4 difference signals) and 2 difference to average signal ratios of MOPITT CO solar channels. The solar channel average and difference signals change almost linearly with surface reflectivity, which varies greatly and is poorly known. The use of difference and average signals ratios greatly reduce the sensitivity to surface reflectivity in the solar region. X is the state vector consisting of CO mixing ratios at a number of selected pressure levels, surface emissivity ϵ_{thm} at CO thermal channels and surface temperature T_s . b is the vector of known parameters such as ancillary data and instrument parameters.

The direct solution of equation (5) is not possible because it is typically ill-conditioned. In practice the problem of finding solution X in equation (5) is often treated as an optimization problem. X is found by minimizing the difference between observation Y and calculation $F(X, b)$ by the forward model. In the maximum likelihood method, *a priori* information about the state vector is also included in the optimization process. Mathematically, solution X is found by minimizing a cost function $J(X)$ given by

$$J(X) = (Y - F(X, b))^t S_e^{-1} (Y - F(X, b)) + (X - X_a)^t S_x^{-1} (X - X_a). \quad (6)$$

Where Y is the measurement vector, and $F(X, b)$ is the calculated signal vector by the forward model. X is the state vector, and X_a is the *a priori* about the state vector. In other words, X_a is what we know about X before the current measurements. S_e is the measurement noise and forward model error covariance matrix. S_x is the expected variance and covariance of X with regard to X_a .

There are many standard minimization techniques to solve equation (6). If $F(X, b)$ is not too nonlinear or a good first guess can be found that will make $F(X, b)$ fairly linear in a local region about a first guess X_0 , then we can expand $F(X, b)$ as a Taylor series about a guess state vector X_0 given by

$$Y = Y_0 + \left. \frac{\partial F}{\partial X} \right|_{X_0} (X - X_0) = Y_0 + K(X) \Big|_{X_0} (X - X_0). \quad (7)$$

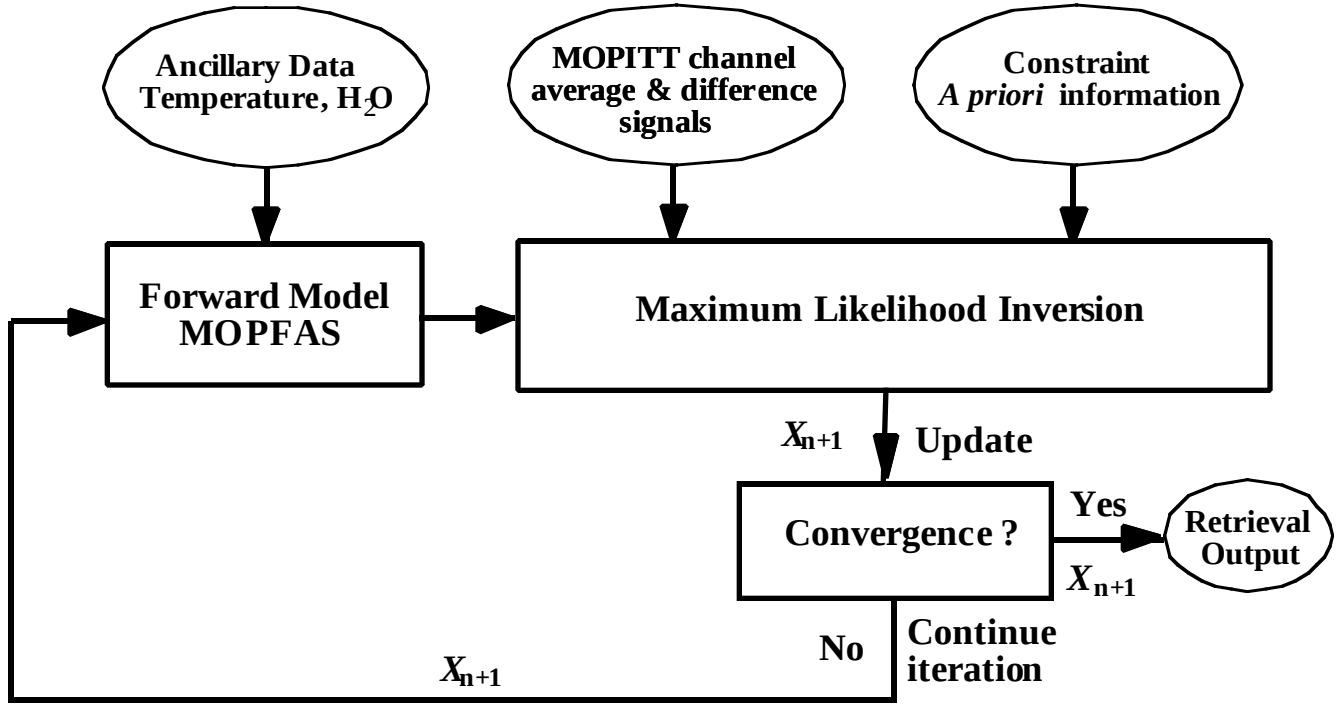


Figure 2. Schematic flow diagram of the operational MOPITT CO retrieval algorithm.

Where high order terms have been neglected based on the assumption that X_0 is not far from the true solution. Y_0 is the calculated signal vector at the first guess X_0 given by $F(X_0, b)$. $\partial F / \partial X = K(x)$ is the Frechet derivative, which is often called the Jacobian. Replacing Y in equation (6) by equation (7) and setting $\partial J(X) / \partial X = 0$, we will get

$$X = X_a + S_X K_{X_0}^T (K_{X_0} S_X K_{X_0}^T + S_\epsilon)^{-1} [Y - Y_0 - K_{X_0} (X_a - X_0)]. \quad (8)$$

Where T stands for matrix transpose. Generally, one iteration is not enough to arrive at the optimum solution. The classical Newton iteration of equation (8) can be used as follows,

$$X_{n+1} = X_a + S_X K_{X_n}^T (K_{X_n} S_X K_{X_n}^T + S_\epsilon)^{-1} [Y - Y_n - K_{X_n} (X_a - X_n)]. \quad (9)$$

The iteration is stopped if a pre-determined convergence criterion is met, such as $X_{n+1} - X_n$ is small enough. As a quality assurance check, $Y_{n+1} - Y_n$ should be smaller or comparable to instrument noise. If $Y_{n+1} - Y_n$ is much bigger than the instrument noise, then solution X_{n+1} is not the optimum solution even though the iteration converges, and should be discarded. One useful characteristics of the maximum likelihood method as shown in (9) is that it also yields error estimates. The error covariance matrix of the solution is given by

$$S = (S_X^{-1} + K_X^T S_\epsilon^{-1} K_X)^{-1}. \quad (10)$$

The operational MOPITT CO retrieval algorithm is illustrated in figure 2. The MOPFAS module calculates the expected MOPITT signals for a particular MOPITT pixel. Inputs to the MOPFAS module include ancillary data and first guess state vector X_0 . Ancillary data includes atmospheric temperature and moisture profiles at standard NASA Data Assimilation Office (DAO) levels, surface pressure, temperature and emissivity, and satellite and solar zenith angles. The maximum likelihood inversion module (equation (9)) generates an updated estimate of the state vector, X_1 . Inputs to the retrieval module include: (1) the calculated signals Y^{cal} ; (2) the MOPITT measured signals in the form of the measurement vector Y^m ; (3) the *a priori* in the form of state vector covariance matrix S_X and first guess X_0 . The updated state vector X_1 is again fed into the MOPFAS

module to generate an updated MOPITT signals calculation Y_1 . The updated calculation Y_1 , the MOPITT measured signal Y^m , and the *a priori* are fed again into the maximum likelihood inversion module to generate a new estimate of the state vector X_2 . The process continues until convergence is achieved. The standard MOPITT retrieval outputs include CO mixing ratios at surface, 850 mb, 700 mb, 500 mb, 350 mb, 250 mb, 150 mb, CO total column, surface temperature T_s , surface thermal channel emissivity ϵ , and error estimates (variances) of each of these variables. The full covariance matrix of the retrieved CO profiles are also available as part of the MOPITT CO retrieval.

4. MOPITT CO RETRIEVAL SIMULATION

The MOPITT CO retrieval algorithm has been tested using simulated MOPITT data before launch. A fairly large ensemble of CO profiles, total of 525 profiles, over diverse geophysical conditions was developed for MOPITT retrieval simulation. It includes CO profile measurements from regular measurement programs, such as NOAA/CMDL trace gas monitoring program at Carr, Colorado and CSIRO trace gas monitoring program at Cape Grim of Australia, and field campaigns, such as the NASA Global Troposphere Experiment (GTE) campaigns. Many of these CO profiles end at about 8-12 km range. We have used model calculations by the NCAR MOZART model¹⁵ to extend the profiles to 0.1 mb, which is the highest level used in MOPFAS calculation. Ancillary temperature and moisture profiles are from NCEP analysis for the locations and time of the CO profiles.

The 525 profiles are divided into a training set containing 263 profiles and a test set containing 262 profiles. Each set contains approximately the same number of CO profiles from each of the field campaigns. CO profiles in the training set and data sources are plotted in figure 3. It is clear from figure 3 that these profiles span a large range in mixing ratio, from less than 100 ppbv to more than 500 ppbv. There are sharp peaks in many CO profiles associated with biomass burning and pollution. For example, CO profiles from the NASA GTE TRACE-A over Africa and South America campaigns show strong CO levels in the lower and middle troposphere. TROPOZ and STRATOZ were conducted primarily in polluted coastal city regions, resulting in high CO values in the boundary layer and lower troposphere. The training set was used as the *a priori* to calculate the CO covariance matrix S_x and a mean CO profile X_a .

The test set was used to generate the simulated MOPITT data. Instrument noises were added to the simulated MOPITT data. The simulated MOPITT data were then used as inputs in the MOPITT CO retrieval simulation. The retrieved CO profiles were compared with the test profiles, and the root-mean-square (RMS) deviation at each of the standard retrieval output pressure levels were calculated. Figure 4 shows the RMS error derived from 262 retrievals using the test set CO profiles. Examples of individual retrievals are plotted in figure 5. The large RMS error in the boundary layer (between 1000 and 900 mb) could be attributed to bias in the *a priori* data set (the training data set), which contains a large number of CO profiles with high CO levels in the boundary layer and lower troposphere from polluted coastal regions and biomass burning regions in Africa and South America.

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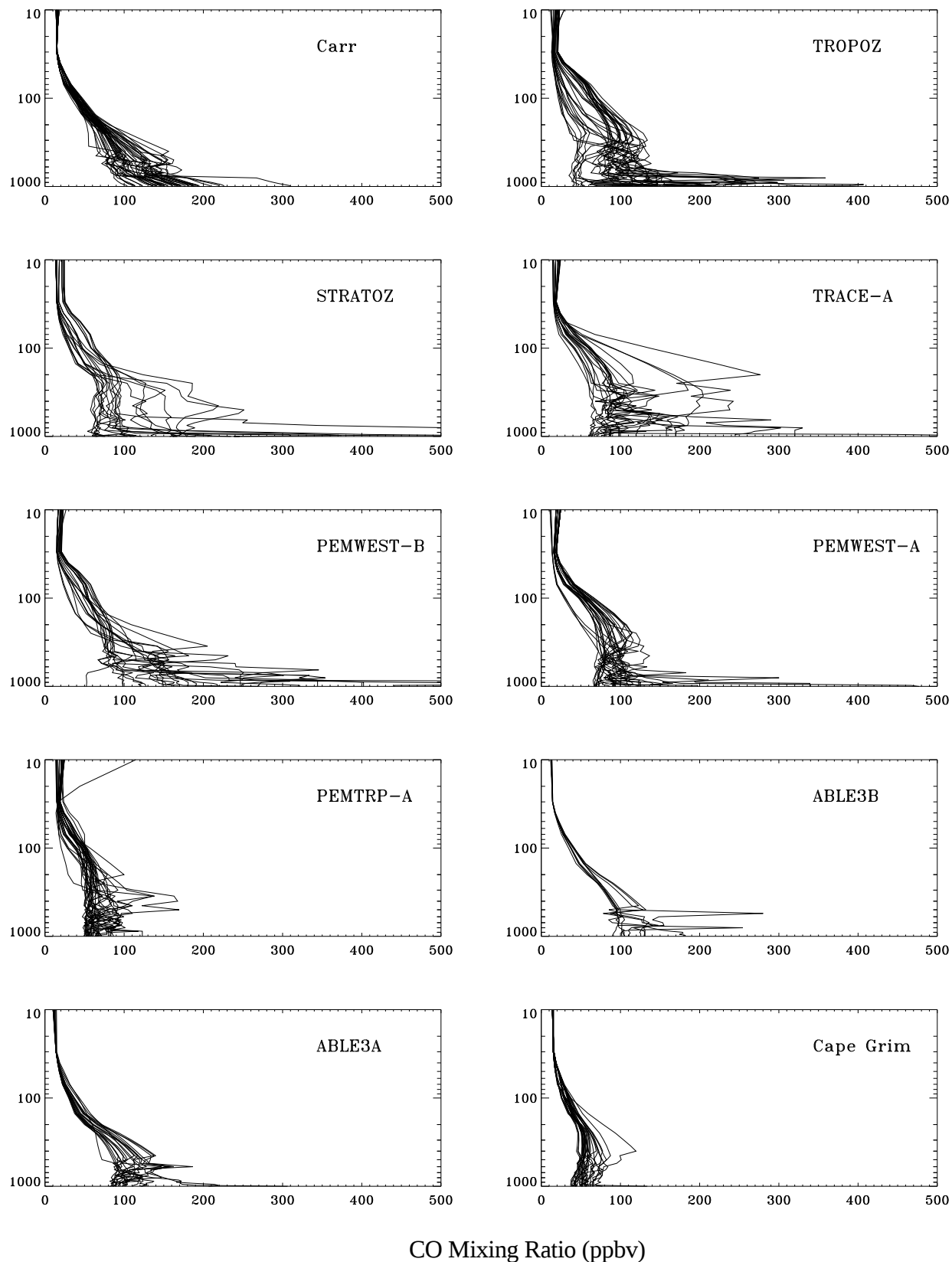


Figure 3. Plots of the training CO profile set used as *a priori* in CO retrieval simulation.

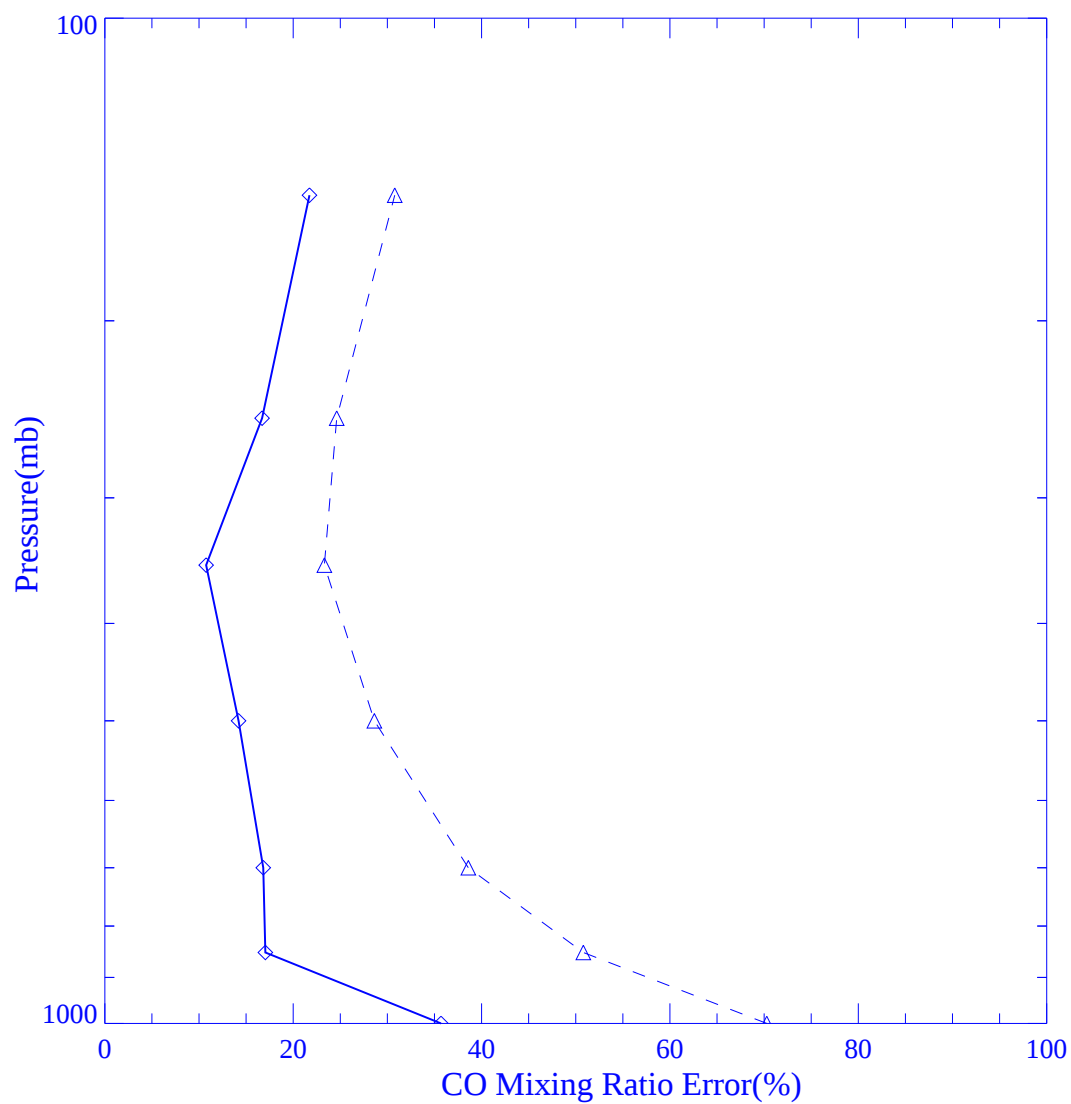


Figure 4. RMS errors of first guess and retrieved CO profiles using simulated MOPITT data. Triangles represent the RMS errors between the first guess and true CO profiles. Diamonds represent the RMS errors between the retrieved CO profiles and true CO profiles, which are used to generate the simulated MOPITT data.

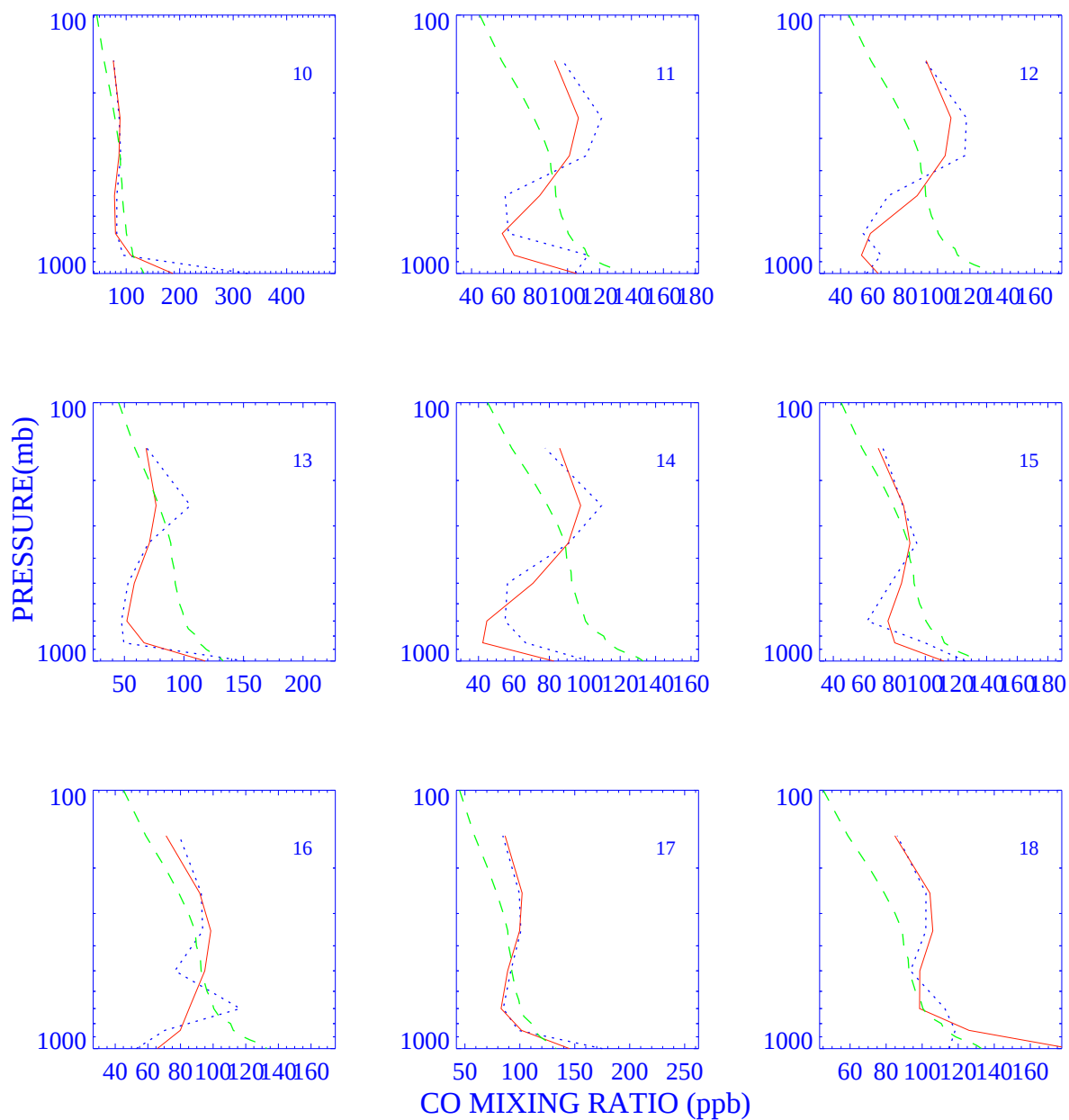


Figure 5. Examples of CO retrievals using simulated MOPITT data. The dotted lines are the true CO profiles from the test set. The dash lines are the first guess, which is the mean of all the CO profiles in the test set. The solid lines are the retrieved CO profiles.

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