MOPITT multispectral CO retrievals: Origins and effects of geophysical radiance errors

M. N. Deeter,1 H. M. Worden,1 J. C. Gille,1 D. P. Edwards,1 D. Mao,1 and James R. Drummond2

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[1] An obstacle to the simultaneous use of near-infrared (NIR) and thermal infrared (TIR) observations from the Measurements of Pollution in the Troposphere (MOPITT) instrument has been a lack of understanding of NIR radiance errors. Retrieval uncertainties produced by optimal estimation-based retrieval algorithms used for satellite instruments like MOPITT are only meaningful if radiance error statistics are accurately quantified in the measurement error covariance matrix. MOPITT’s gas correlation radiometers are subject to a unique form of “geophysical noise” due to the combined effects of (1) translational motion of the instrumental field of view during a single observation and (2) fine-scale spatial variability of surface radiative properties. We describe and demonstrate a new method for quantifying this source of error for each observation. Both TIR and NIR radiance errors due to this effect are highly variable, especially over land, but are qualitatively consistent with the variability of Moderate Resolution Imaging Spectroradiometer radiances in similar spectral bands. In addition, retrieval algorithm modifications are described which adjust the trade-off between smoothing error and retrieval noise within the optimal estimation framework. These modifications are necessary to fully exploit the information in MOPITT’s NIR channels. A case study based on MOPITT observations over Minnesota demonstrates significant improvement in retrieval performance as the result of the retrieval algorithm modifications.


1. Introduction

[2] The Measurements of Pollution in the Troposphere (MOPITT) instrument on the Earth Observing System Terra platform has now acquired more than ten years of global carbon monoxide (CO) observations, forming the longest satellite record for an important atmospheric pollutant. MOPITT CO products have been thoroughly validated [Emmons et al., 2009] and are routinely exploited to quantify CO emissions [Kopacz et al., 2009; Fortems-Chiney et al., 2011], analyze long-range transport of pollution [Edwards et al., 2006], and evaluate chemical transport models [Shindell et al., 2006].

[3] MOPITT is uniquely equipped with both thermal infrared (TIR) and near-infrared (NIR) gas correlation radiometers [Drummond, 1992]. This multispectral capability of MOPITT was intended to permit the retrieval of lower tropospheric CO concentrations, which is advantageous to applications including air quality monitoring [Clerbaux et al., 2008; Kar et al., 2010] and inverse modeling [Kopacz et al., 2009; Fortems-Chiney et al., 2011]. MOPITT TIR observations, like the measurements made by the AIRS [McMillan et al., 2005], TES [Rinsland et al., 2006], and IASI [George et al., 2009] instruments, are sensitive to midtropospheric and upper tropospheric CO concentrations, except in strong thermal contrast conditions in which lower tropospheric CO becomes radiatively significant [Deeter et al., 2007]. MOPITT NIR observations, like those of SCIAMACHY [de Laat et al., 2007], are relatively insensitive to the vertical distribution of CO and effectively constrain the integrated total column [Deeter et al., 2009]. Conceptually, CO concentrations in the lower troposphere can be determined from the difference between the retrieved CO total column (NIR information) and the retrieved partial column representing the midtroposphere and upper troposphere (TIR information). Thus, for the purpose of retrieving lower tropospheric concentrations of CO, MOPITT’s TIR and NIR observations are complementary.

[4] However, until recently, complex geophysical noise processes affecting the NIR radiances prevented their use in operational MOPITT retrieval products. Details of these processes are described below. Thus, the current MOPITT “Version 4” product exploits the TIR radiances only. Early
attempts to exploit MOPITT’s NIR channels were unsuccessful due to a low rate of retrieval convergence and large random errors in the retrieval results. In the first demonstrated use of MOPITT’s CO NIR observations, geophysical noise was assumed to be correlated with instrumental noise [Deeter et al., 2009]. More recently, retrieval results based on both MOPITT TIR and NIR observations were demonstrated for the first time [Worden et al., 2010]. In both of these studies, however, the underlying physical source of the geophysical noise was not analyzed.

[6] Recently, our quantitative understanding of geophysical noise processes has significantly advanced. Because MOPITT is stationed on a polar-orbiting platform, its field of view travels a finite distance during the time interval required to make a single observation. This motion, combined with subpixel variability of the surface radiative properties (e.g., surface reflectance and surface temperature), results in radiance errors substantially greater than the instrumental noise.

This effect is described further in Section 3.1. MOPITT data processing algorithms have been adapted to quantify and rigorously account for these radiance errors in the production of new NIR and joint TIR/NIR retrieval products. The methods described in this manuscript will be embodied in the new MOPITT “Version 5” retrieval products.

2. MOPITT Measurement Principles

[6] Gas correlation radiometers employ internal gas-filled cells that act as modulated high spectral resolution optical filters. The cells are filled with the “target gas” (i.e., the atmospheric gas to be measured) and are coupled to mechanisms which modulate either the optical path length through the absorbing gas or the cell pressure. Such devices are known as length-modulated radiometers (LMRs) and pressure-modulated radiometers (PMRs), respectively [Drummond, 1992; Tolton and Drummond, 1997]. When combined with a means for calibration, a gas correlation radiometer produces two radiances characterized by complementary spectral transmittance profiles. Within a broad spectral envelope defined by a spectral bandpass filter, these systems independently measure radiation (1) in the spectral gaps or windows between the absorption lines of the target gas (the Average or A radiances) and (2) in narrow spectral regions containing the absorption lines of the target gas (the Difference or D radiances) [Drummond, 1992; Edwards et al., 1999]. D radiances are typically much more sensitive to atmospheric concentrations of the target gas than A radiances, which are used to characterize the background signal. Both the A and D radiances contain necessary information for retrieving CO, and are therefore complementary. For the NIR radiances, the ratio D/A is employed in the retrieval algorithm as a means of canceling the first-order effects of surface reflectance variability [Pan et al., 1998]. This cancelation is exact for homogeneous surfaces exhibiting spectrally uniform surface properties [Deeter et al., 2009]. More generally, surface heterogeneity and surface reflectivity spectral variability can both introduce errors in the ratio D/A.

[7] The MOPITT instrument includes four LMRs (two of which contain methane, and are not discussed further) and two PMRs. An instrument malfunction in May 2001 resulted in the permanent loss of two LMRs (one CO LMR and one methane LMR) and one PMR. The remaining PMR measures CO in the 4.7 μm fundamental band (Channel 7), while the remaining CO-filled LMR measures CO at both 4.7 μm (Channel 5) and at the 2.3 μm first overtone band (Channel 6). Properties of these three MOPITT channels are summarized in Table 1. Each LMR alternately passes the radiation from Earth through a Long (L) and Short (S) gas path, thereby modulating the absorption by the target gas. As indicated in Figure 1, digitized optical detector counts are recorded at each L and S state of the LMR. A total of 16 Level 0 digitized counts acquired during eight full L-S cycles are used to produce a single MOPITT Level 1 radiance (i.e., one MOPITT observation). Similarly, counts from the PMR are recorded during the two opposite phases of the pressure modulation cycle (but are characterized by High and Low states instead of the LMR’s L and S states).

[8] During the calibration of a single LMR observation, the 16 raw counts, part of the Level 0 Product, are processed into an A radiance and a D radiance for each channel. A radiances for the LMR are derived from the mean of the Land S counts, whereas D radiances are derived from the difference of the L and S counts. The calibrated radiances are reported in the MOPITT Level 1 Product along with corresponding uncertainty values and geolocation information. To convert from counts to radiance values, the calibration process exploits periodic views of space (as a reference for zero radiance) and an internal blackbody target with known temperature and emissivity [Deeter et al., 2002]. For V3 and V4 MOPITT products, the space view Level 0 data were also used as the basis of instrument noise calculations (as discussed below). The remaining LMR and PMR thus yield three pairs of A and D radiances from which to retrieve the CO profile. Channel 5 radiances (5A and 5D) are produced by the 4.7 μm (TIR) LMR. Radiances 6A and 6D are produced by the 2.3 μm (NIR) LMR. Radiances 7A and 7D are produced by the 4.7 μm (TIR) PMR.

3. Radiance Error Sources and Estimation

[9] The maximum a posteriori (MAP) solution \( \hat{x}_{\text{MAP}} \) provides the basis of the MOPITT retrieval algorithm [Rodgers, 2000; Deeter et al., 2003]. Mathematically, it may be written

\[
\hat{x}_{\text{MAP}} = x_a + G_{\text{MAP}}(y - Kx_a)
\]

where

\[
G_{\text{MAP}} = C_oK^T(KC_oK^T + C_i)^{-1}
\]

and where \( x_a \) is the a priori state, \( C_o \) is the a priori covariance matrix, \( K \) is the weighting function matrix (which describes the forward model–calculated sensitivity of the each of the measurement vector elements to each of the elements of the state vector), \( y \) is the measurement vector and \( C_i \) is the measurement error covariance matrix. The gain matrix \( G_{\text{MAP}} \) describes the sensitivity of the retrieval to the measurement. The corresponding retrieval error covariance matrix for the MAP solution is

\[
C_x^{\text{MAP}} = (K^T C_o^{-1}K + C_i^{-1})^{-1}
\]
With respect to the retrieval algorithm, radiance errors are defined as differences between actual measured (calibrated) radiances and corresponding model-calculated radiances for a scene represented by known geophysical parameters. Radiance errors, which may be either random or systematic, may be associated with the instrument, the forward radiative transfer model, or geophysical effects. Properly representing the statistical variability of these radiance errors in the form of a measurement error covariance matrix is an essential requirement of optimal estimation. Previously, the measurement error covariance matrix $C_1$ was assumed to be the sum of two matrices separately representing instrument noise and forward model error, i.e.,

$$C_1 = C_y + C_f$$

where $C_y$ is the instrument error covariance matrix and $C_f$ is the forward model error covariance matrix [Deeter et al., 2003]. For the MOPITT V3 and V4 products, diagonal elements of $C_y$ were determined through the analysis of the variability of Level 0 counts recorded while the MOPITT scanning mirror was periodically pointed to space. Off-diagonal elements of $C_y$ were assumed to be zero, since electronic noise processes should be uncorrelated for different channels. Moreover, it was assumed that the instrument noise was independent of the background scene, i.e., space view instrument noise values were assumed to be equally valid regardless of whether the instrument was viewing space or the Earth. Elements of $C_f$ were previously determined by comparing radiances produced by MOPFAS (the fast operational radiative transfer model) and an accurate “benchmark” radiative transfer model known as MOPABS [Edwards et al., 1999]. This matrix includes both diagonal and off-diagonal nonzero elements.

### 3.1. LMR Radiances

For the LMR channels, consecutive L and S counts are recorded 25 ms apart while the instantaneous field of view (IFOV) travels continuously over the Earth’s surface (see Figure 1). Both NIR and TIR LMR measurements are affected by surface characteristics. For NIR measurements, Level 0 counts are proportional to the mean surface reflectance averaged over the IFOV. For TIR measurements, Level 0 counts are sensitive to both the surface temperature and surface emissivity averaged over the IFOV. Thus, because the IFOV samples 16 distinct (but overlapping) scenes for any given MOPITT pixel, spatial variability of the physical characteristics of the surface results in fluctuations in the set of Level 0 L and S counts that are used to calculate a single radiance. Statistically, these fluctuations reduce the precision with which the $A$ and $D$ radiances can be calculated. While these fluctuations are not truly random, as they often are for instrumental noise processes, they produce the same effect on the calibrated radiances; thus we use the term “geophysical noise” for this effect.

Geophysical noise is demonstrated further in Figure 2, where actual Channel 6 Level 0 L counts for a single detector element are plotted versus time. (S counts are not shown for clarity; the effects of geophysical noise are equally evident for the L and S counts.) The data were recorded starting at 19:14:35 UTC on 4 September 2004 as MOPITT’s field of view scanned over a track beginning over the Pacific Ocean.
and ending over Northern California. Each group of eight consecutive L counts (plotted as black plus signs) represent a single MOPITT pixel; Figure 2 presents Level 0 data for fifteen pixels over ocean and land. The approximate time at which the field of view crossed the California coastline is depicted by the vertical dashed line. Standard deviations for each group of 8 counts, representing the geophysical noise, are indicated by purple diamonds. Vertical axes on the left and right sides of the plot correspond to the actual counts and the standard deviations, respectively.

[13] As the MOPITT field of view approaches and crosses the coastline, the counts increase as the result of increasing surface albedo. This transition occurs gradually over several MOPITT pixels, perhaps as the result of either decreasing ocean depth or increasing foam coverage from breaking waves. Standard deviations over land are clearly much larger than for open ocean, indicating greater subpixel variability of surface reflectance. For example, the mean standard deviation for the first six oceanic pixels is 284 counts whereas the mean standard deviation for the last three overland pixels is 9189 counts. Figure 2 also shows that standard deviation values are highly variable over land and even in the coastal region. Over land, we suspect that land use patterns, variations in vegetation, and solar illumination differences caused by topography might all contribute to large differences in standard deviations from one pixel to the next.

[14] Radiance errors introduced by surface reflectance spatial variability can be understood by considering how different spatial frequencies in the surface reflectance Fourier decomposition (or spatial spectrum) affect the different spatial frequencies in the surface reflectance. For example, surface reflectance variability at the spatial frequency \( f_0 \) defined by the full cycle between consecutive L or S measurements (a distance of approximately 336 m) produces the largest potential error on the calibrated \( D \) radiances (compared to other spatial frequencies). This spectral component has no effect on the calibrated \( A \) radiances, however, since it has no effect on the sum of the L and S counts. In contrast, surface reflectance variability at the spatial frequency \( 2f_0 \) acts as a source of error for the \( A \) radiances but not the \( D \) radiances.

[15] As described previously [Deeter et al., 2009], the MOPITT Level 1 Processor includes a correction involving each “triplet” of three consecutive LMR Level 0 counts. The complete set of 16 counts (8 L and 8 S) for a single LMR Earth view observation yields 14 triplets. For each triplet, both an Average and a Difference count are calculated. The actual \( A \) and \( D \) radiances for each LMR observation are determined by averaging the \( A \) and \( D \) counts over all 14 triplets and applying calibration to convert from counts to radiances [Deeter et al., 2002]. The triplet method should effectively remove the first-order effect of surface reflectance spatial variability (i.e., the very lowest spatial frequencies) but will not affect the component at \( f_0 \) or higher spatial frequencies.

[16] To explicitly represent the effects of geophysical noise on the radiance uncertainties, the instrument error covariance matrix \( C_y \), in equation (4) has been replaced with the more general “observation error covariance matrix” \( C_{obs} \); this matrix represents the combined effects of instrumental noise and geophysical noise. Hereafter, we use the term “observation-dependent noise” (or O.D. noise) to refer to the cumulative noise resulting from combined instrumental and geophysical sources. Like \( C_y \), \( C_{obs} \) is assumed to be a diagonal matrix; i.e., geophysical radiance errors are assumed to be uncorrelated between channels. (Potential cross-channel geophysical noise correlations will be investigated in future studies.) However, whereas elements of \( C_y \) for V3 and V4 were strictly based on space view counts, elements of \( C_{obs} \) are based on the variability of the triplets that make up individual Earth view observations. Specifically, diagonal elements of \( C_{obs} \) for the four LMR radiances (5A, 5D, 6A, and 6D) are set equal to the standard deviations of the 14 triplet-based \( A \) and \( D \) values. Thus, scenes characterized by greater surface heterogeneity yield larger \( C_{obs} \) values than scenes which are relatively homogeneous. Since the triplet variability for each observation represents both instrument noise and geophysical noise, there is no need to actually calculate instrumental noise and geophysical noise as separate components.

3.2. PMR Radiances

[17] Unlike the LMR calibrated radiances, which are based on multiple L and S counts within each observation, the Level 0 data that make up each PMR Earth view observation consist of a single high-pressure (H) count and a single low-pressure (L) count. Statistically, it is therefore impossible to use Earth view Level 0 data for individual PMR Earth view observations to estimate the geophysical noise corresponding to radiances \( 7A \) and \( 7D \). Elements of \( C_{obs} \) corresponding to \( 7A \) and \( 7D \) are thus determined using space view Level 0 data only, in the same manner as for the V3 and V4 Level 1 products. Retrieval results presented here (as well as the V3 and V4 products) exploit the \( 7D \) radiance but not the \( 7A \) radiance.

4. Observed Radiance Error Variability

[18] O.D. noise values for 5A, 5D, 6A and 6D radiances were calculated for all clear-sky MOPITT observations acquired during September 2004. The values were then normalized by the corresponding instrument-only noise values and gridded at 0.5 degree latitude/longitude resolution. As shown by the gridded monthly mean O.D. noise maps presented in Figure 3 (5A and 5D) and Figure 4 (6A and 6D), normalized O.D. noise values over North America vary by up to several orders of magnitude. The clear geographical dependence of the O.D. noise values evident in Figures 3 and 4 indicates a geophysical source. According to the arguments presented in Section 3 and the results presented in Figure 2, O.D. noise values depend on the heterogeneity of surface properties (e.g., surface reflectance for NIR measurements, surface temperature and emissivity for TIR measurements) at scales smaller than the MOPITT footprint. In turn, the fine-scale spatial variability of these physical properties likely depends on topographic variability as well as the heterogeneity of soil composition, vegetation, bodies of water, and other surface characteristics.

[19] Examination of Figures 3 and 4 shows that normalized O.D. values over the ocean tend to be uniformly small (near unity) for the 5A, 5D, 6A, and 6D radiances. As normalized O.D. values approach unity, geophysical noise becomes negligible compared to instrumental noise. In contrast, O.D.
noise values over land are typically greater than values over ocean, but are highly variable. Normalized O.D. noise values for the NIR radiances reach much greater values over land than for the TIR radiances, but are significantly greater than unity for both. For all four radiances, O.D. noise values tend to be much larger in the Western U.S. than the Eastern U.S. and appear particularly large over the Central Rocky Mountain region (e.g., the region bounded by 35N, 40N, 110W and 105W). Factors which might explain the larger O.D. noise values in the Western U.S. include (1) greater topographical variability, which produces subpixel variations in solar illumination, and (2) sparser vegetation (and thus more exposed rock and bare soil). O.D. noise values are particularly low in the U.S. Upper Midwest (e.g., the region near 43N and 95W).

[20] The observed geographical variability of O.D. noise has been compared with observations made by the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument which is also on the Terra satellite and like MOPITT makes observations in both NIR and TIR spectral bands. The much smaller size of the 1 km MODIS footprint compared to the 22 km MOPITT footprint allows a qualitative analysis of the effects of subpixel surface reflectance heterogeneity on MOPITT O.D. noise. MODIS Band 7 measures NIR radiances in the spectral interval 2.105 to 2.155 μm, similar to the passband between 2.22 to 2.31 μm for MOPITT Channel 6 [Edwards et al., 1999]. MODIS Band 23 measures integrated TIR radiances in the spectral interval 4.020 to 4.080 μm, which is near the passband for MOPITT Channel 5 [Edwards et al., 1999]. (MODIS Bands 24 and

**Figure 3.** Monthly mean normalized 5A and 5D (TIR) O.D. noise values over North America for September 2004.
25 are spectrally closer to MOPITT’s TIR passband for Channel 5 than Band 23, but are characterized by much higher atmospheric absorption.

[21] For the same geographical area shown in Figures 3 and 4, clear-sky MODIS 1 km resolution radiances for Bands 7 and 23 observed on 14 September 2004 were arbitrarily binned at 0.25 degree latitude/longitude resolution. MODIS radiance standard deviations, which serve as an index for surface reflectance spatial variability, were then calculated for each grid cell and are presented in Figure 5. Qualitatively, the large-scale patterns evident in the MOPITT O.D. noise maps are similar to the patterns in the maps of MODIS radiance variability. Like the MOPITT O.D. noise values, MODIS radiance variability is typically larger and more variable over land than over ocean. Over land, both MOPITT O.D. noise values and MODIS radiance variability are both sharply higher in the Western U.S. compared to the Eastern U.S. Thus, for both TIR and NIR observations, comparisons between MOPITT O.D. noise values and MODIS radiance variability support the hypothesis that O.D. noise results from subpixel variability of surface properties combined with field of view motion.

5. Retrieval Algorithm Modifications

[22] In order to amplify the sensitivity of the retrieved profiles to the NIR radiances, both previous efforts to exploit MOPITT’s NIR CO channels [Deeter et al., 2009; Worden et al., 2010] underestimated the effect of geophysical noise and assumed the noise to be fixed for all
observations. In the paper by Deeter et al. [2009], geophysical noise was estimated by simply scaling the pure instrumental noise by a factor of five. In the paper by Worden et al. [2010], O.D. noise variance was modeled as the sum of the purely instrumental noise variance and a small constant term representing geophysical noise.

As shown below, the representation of O.D. noise in the retrieval algorithm directly affects the relative magnitudes of retrieval noise and smoothing error. Smoothing error, represented by the smoothing error covariance matrix $C_s$, describes the expected errors between the true profile and retrieved profile due to the characteristics of the weighting functions and influence of the a priori covariance matrix. Retrieval noise, represented by the retrieval noise covariance matrix $C_n$, quantifies the expected errors due to errors in the radiances. $C_s$ and $C_n$ can be obtained from the equations

$$C_s = (I - GK)C_a(I - GK)^T$$

and

$$C_n = GC_aG^T$$

The sum of $C_s$ and $C_n$ yields the retrieval error covariance matrix $C_x$, i.e.,

$$C_x = C_s + C_n$$

**Figure 5.** Clear-sky MODIS radiance standard deviations for Bands 7 and 23 gridded at 0.25 degree latitude/longitude resolution for daytime overpasses on 11 September 2004. Cloudy MODIS radiances were excluded through application of the MODIS cloud mask.
The chosen value of $\gamma$, which controls the desired tradeoff between smoothing error and retrieval noise, primarily involves two considerations. First, if the product $\gamma C_r$ in equation (9) is taken to represent the measurement error covariance matrix for an ensemble of $N$ independent measurements dominated by random error, setting $\gamma$ to $N^{-1}$ would actually yield the optimal MAP solution for the ensemble average (since random noise variance values decrease as $N^{-1}$). Thus, a reasonable choice for $\gamma$ might simply be $N^{-1}$, where, for example, $N$ might be the typical number of MOPITT retrievals in a 1 degree by 1 degree latitude/longitude box (the grid cell size for MOPITT Level 3 products). In this case, potential values of $N$ would range from 1 (for a nearly completely cloud-filled grid cell) to a maximum of about 25 (a completely clear grid cell). The corresponding range of possible $\gamma$ values would be 1 and 0.04.

An important and more practical consideration with respect to $\gamma$ concerns retrieval stability. As $\gamma$ decreases, retrievals become progressively more unstable; an increasing fraction of retrievals fail due either to nonconvergence (excessive iterations) or incompatibility with the operational forward model [Deeter et al., 2010]. In the V4 product, daily retrieval failure rates typically vary between 0.2% and 2.0%. Allowing significantly higher fractions of retrievals to fail should be avoided since it would reduce retrieval coverage and possibly introduce retrieval bias.

6. Averaging Kernel Comparisons

New data processing software was developed to implement and exploit (1) observation-dependent noise values for all of the LMR radiances (as described in Section 3.1) and (2) the suboptimal variation of the MAP solution (as described in Section 5). MOPITT observations for 4 August 2010 were then processed using three different retrieval algorithm configurations. The first configuration exploited only the TIR radiances (7D, 5A, and 5D) with $\gamma$ set to 1.0. This configuration is comparable to the MOPITT V4 product, except that the V4 product does not account for geophysical noise. The second and third configurations both exploited the TIR and NIR radiances (6D and 6A), but with two different values of $\gamma$: 1.0 (the MAP solution) and 0.2. Smaller values of $\gamma$ were not investigated because of observed decreases in retrieval convergence. For example, in rare cases, retrieval failure rates approaching 50% were observed when $\gamma$ was set to 0.05.

Figure 6 (top) presents mean surface level averaging kernels and (bottom) DFS histograms for MOPITT observations of central Minnesota processed for three contrasting retrieval configurations.

Underestimating the uncertainties in the measurements (as was done previously) tends to reduce smoothing error while increasing retrieval noise. Moreover, this method leads to artificially small estimates of retrieval noise as calculated according to equation (6). While the two earlier papers clearly demonstrated the potential value of MOPITT’s NIR observations, neither of these papers described a method for calculating reliable retrieval uncertainties for NIR-based products. The provision of robust retrieval uncertainties is a first-order requirement for MOPITT retrieval algorithm development.

Conceptually, the MAP solution defined in equation (1) minimizes $C_x$ for each individual observation [Rodgers, 2000]. However, users of satellite data sets like the MOPITT CO product commonly exploit large ensembles of retrievals. Such users frequently average the MOPITT retrieval data spatially and/or temporally, which substantially reduces the effects of random radiance errors (retrieval noise) but does not reduce smoothing error. Thus, retrieval averaging does not increase the retrieval sensitivity. This suggests that users of ensembles of MOPITT retrievals would benefit if the retrieval sensitivity were increased, even at the expense of higher retrieval noise. As demonstrated in Section 6, this strategy results in greater sensitivity of the retrievals to the NIR radiances and specifically increases the sensitivity to surface level CO.

A method for adjusting the balance between retrieval noise and smoothing error in the context of optimal estimation is described in Chapter 4 of Rodgers [2000]. The method increases the gain matrix $G$ by introducing a gain enhancement factor $\gamma$ that scales $C_r$ in equation (2). The resulting solution $\hat{x}^{SO}$ is “suboptimal” in the sense that, unlike the MAP solution, it does not minimize the expected difference between the true state and the retrieved state for each individual observation. The solution is simply

$$\hat{x}^{SO} = x_0 + G^{SO}(y - Kx_0)$$

where

$$G^{SO} = C_r K^T (K C_r K^T + \gamma C_x)^{-1}$$

As $\gamma$ approaches unity, $\hat{x}^{SO}$ approaches the MAP solution $\hat{x}^{MAP}$. As $\gamma$ decreases, $G^{SO}$ increases, i.e., the retrieval sensitivity (and averaging kernels) increase relative to the MAP solution.

Figure 6. (top) Comparison of mean surface level averaging kernels and (bottom) DFS histograms for MOPITT observations of central Minnesota processed for three contrasting retrieval configurations.
47N, 96W and 94W) for the three retrieval configurations just described. For both the TIR-only and TIR/NIR (γ = 1.0) configurations, $A_{\gamma/c}$ peaks near 700–800 hPa and decreases sharply toward the surface. Thus, for the standard MAP solution (γ = 1.0), inclusion of the NIR radiances does not significantly increase the sensitivity to CO in the lower troposphere in this scene. In contrast, results for the suboptimal TIR/NIR (γ = 0.2) configuration indicate significantly better sensitivity to CO near the surface. Other geographical regions exhibit similar improvements in $A_{\gamma/c}$ using suboptimal values of γ, although a variety of factors (such as thermal contrast conditions, mean surface albedo and surface heterogeneity) affect the magnitude of the improvement. Histograms of Degrees of Freedom for Signal (DFS) are presented in Figure 6 (bottom) for the same scene in Minnesota. Mean DFS values for the TIR-only, TIR/NIR (γ = 1.0), and suboptimal TIR/NIR (γ = 0.2) configurations are 1.377, 1.427, and 1.841, respectively. Similar to the results for $A_{\gamma/c}$, retrievals processed with γ set to 1.0 are thus only slightly improved by the NIR radiances. For TIR/NIR retrievals, reducing γ from 1.0 to 0.2 increases the mean DFS value by 0.414.

7. Conclusion

Several key trace gases lend themselves to remote sensing methods in multiple spectral regimes. For example, both NIR- and TIR-based methods have been developed for retrieving carbon monoxide, carbon dioxide, methane and water vapor. In principle, observations in different spectral regimes are characterized by different vertical weighting functions and therefore yield independent constraints on the retrieved vertical profile. However, while these fundamentally different types of observations are clearly complementary, very few satellite instruments have actually been designed to exploit this multispectral synergy. MOPITT, for example, is currently the only satellite instrument able to make simultaneous NIR and TIR observations of CO. MOPITT was designed with this feature specifically to increase the sensitivity to CO in the lower troposphere, where major sources lie. Thus, applications including air quality monitoring [Clerbaux et al., 2008; Kar et al., 2010] and inverse modeling [Kopacz et al., 2009; Fortems-Cheiney et al., 2011] should benefit from the availability of MOPITT multispectral retrieval products.

The main obstacle to merging MOPITT’s TIR and NIR observations in a single retrieval product has been a lack of understanding of NIR radiance errors. Over land in particular, it is now evident that the combined effects of field of view motion and subpixel variability in surface characteristics produce effectively random geophysical radiance errors which are often much larger than instrumental errors. (An instrument with a fixed field of view should not suffer from this effect. This design feature could be achieved either through satellite motion compensation, as has been discussed for a possible MOPITT follow-on mission, or by stationsing the instrument in a geostationary orbit as envisioned for the GEO-Cape platform [Edwards et al., 2009].) Neglecting this geophysical noise in the MOPITT retrieval algorithm leads to retrieval nonconvergence problems and prevents meaningful retrieval error estimation.

A method for quantifying this geophysical noise term for each observation made by MOPITT’s LMRs has been developed and implemented in data processing software. These changes are incorporated into new MOPITT Version 5 (V5) retrieval products. Based on the analysis of one month of observations over North America, geophysical noise varies over a wide range but is typically much larger over the Western U.S. than the Eastern U.S. These findings are qualitatively consistent with analyses of MODIS radiance spatial variability. More analysis will be required to fully understand how geophysical noise varies geographically and temporally.

When exploited within the standard optimal estimation-based retrieval algorithm, geophysical noise in MOPITT’s NIR radiances often yields weak retrieval sensitivity to CO in the lower troposphere. Multispectral retrievals based on TIR and NIR radiances do not necessarily offer better retrieval performance than pure TIR-based retrievals. This problem has been circumvented by introducing a “gain enhancement factor” in the optimal estimation retrieval algorithm which effectively reduces retrieval smoothing error at the expense of increasing retrieval noise. This modification affects the retrieval error covariance matrix (as well as the retrieval itself), and yields retrieval uncertainties which fully quantify the combined effects of smoothing error and retrieval noise. New V5 retrieval products based on this modified algorithm are appropriate for users who tend to exploit spatial ensembles of retrievals rather than isolated individual retrievals. For a case study based on observations over Minnesota, the surface level sensitivity for TIR/NIR retrievals improves significantly as the result of the described algorithm modifications.

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M. N. Deeter, D. P. Edwards, J. C. Gille, D. Mao, and H. M. Worden, Atmospheric Chemistry Division, National Center for Atmospheric Research, Boulder, CO 80307, USA. (mnd@ucar.edu)
J. R. Drummond, Department of Physics and Atmospheric Science, Dalhousie University, Halifax, NS B3H 3J5, Canada.