Retrieval of tropospheric methane from MOPITT measurements: algorithm description and simulations

Merritt N. Deeter*, Jinxue Wang, John C. Gille, and Paul L. Bailey

National Center for Atmospheric Research, P.O. Box 3000, Boulder, CO 80307-3000

ABSTRACT

Tropospheric concentrations of methane have been increasing at a rate of approximately 1% / year, though recent measurements suggest some slowing in this trend. Increased concentrations of methane, a greenhouse gas, will have significant consequences for tropospheric chemistry and climate on a global scale. Characterization of the spatial and temporal variability of methane is one goal of the MOPITT (Measurement of Pollution In The Troposphere) instrument included on the EOS Terra satellite. This instrument includes spectral channels designed to measure methane total column with approximately 1% precision with a spatial resolution of approximately 22 x 22 km.

Retrieval of the methane total column will be accomplished by the MOPITT instrument from measurements of solar radiation reflected at the earth's surface. Gas correlation radiometry will be used to separate the spectral signature of methane in the upwelling radiance from features produced by other trace gases. The retrieval algorithm is based on maximum likelihood and uses an initial guess profile and methane total column variance estimates provided by aircraft in-situ measurements. In this talk, we will describe features of the retrieval algorithm in detail and present results of retrieval simulations conducted to test the sensitivity of the retrieval algorithm to various sources of error.

Keywords: Carbon monoxide, methane, remote sensing, MOPITT, retrieval algorithm, maximum likelihood

1. INTRODUCTION

Methane is an important trace gas in the troposphere, both because of its role in atmospheric chemistry and because of its role as a greenhouse gas.[1] Methane concentrations in the atmosphere have increased sharply during most of this century, although measurements made this decade indicate some stabilization.[2] Methane sources include wetlands, tropical rain forests, livestock, and agriculture. Currently, however, there are no operational remote sensing methods for measuring methane concentrations with global coverage. Such measurements would be particularly useful in geographical areas where in-situ measurements are currently rare, such as over the oceans and polar regions. Both global chemistry models and climate models should benefit greatly from increased frequency and coverage of methane observations.

The MOPITT instrument is included among several remote sensing instruments mounted on the EOS Terra satellite (formerly known as AM1), currently scheduled for launch during the summer of 1999.[3] The MOPITT instrument design exploits gas correlation radiometry, which is a technique for using gas cells to effectively filter the radiatively-active portions of the spectrum for a particular 'target' gas species from 'background' radiation unrelated to the particular species under investigation. Gas cells containing both carbon monoxide and methane are integrated into the MOPITT instrument, with the goal of independently retrieving both the carbon monoxide atmospheric profile and the methane total column (i.e. total number of molecules per unit area in an atmospheric column between the satellite and Earth). This paper describes the operational method for retrieving the methane total column and presents results of numerical retrieval simulations (a companion paper by Wang et al describes the carbon monoxide retrievals).

For redundancy, MOPITT includes two identical length-modulated methane gas correlation cells for the purposes of retrieving methane total column. A broadband optical filter with peak transmittance around 2.2 micron is used to select a

* Correspondence: Email: mnd@eos.ucar.edu; Telephone 303 497-8063; Fax 303 497-2920

band of upwelling radiation spanning a group of methane absorption lines.[4] Demodulation of the electrical signals produced by the photodetectors yields two signals. The methane 'Average' signal S_A corresponds approximately to the intensity of upwelling radiation between the methane absorption lines whereas the methane 'Difference' signal S_D preferentially represents the intensity of upwelling radiation within the methane absorption lines.

2. RETRIEVAL ALGORITHM

The MOPITT retrieval algorithm for methane total column is based on the principle of maximum likelihood described by Rodgers.[5] In essence, the retrieved methane total column is a weighted average of the a priori (climatological) value and the value derived solely from the measured radiances. The relative weights of the two values depends, among other things, on the statistical uncertainty in the measured radiances and the a priori variance of the methane total column. Conceptually, the retrieval algorithm can be described in terms of the retrieval inputs, the forward model, and the maximum likelihood inversion.

2.1. Retrieval Inputs

The retrieval inputs can be divided into categories of MOPITT radiance data, methane a priori data, and ancillary data. Radiance inputs include estimated radiance errors as well as the actual measured radiance values. Radiance errors may include contributions from instrumental sources, the forward model, and errors in the forward model ancillary inputs, such as the atmospheric water vapor profile. The methane a priori includes the a priori methane profile (typically the climatological mean profile) and the statistical variance of the methane total column. These data are typically generated by statistical analysis of large sets of in-situ measured profiles. The ancillary data includes both the surface values and the atmospheric profile information which, along with a methane vertical profile, are required to execute the forward radiative transfer model. Required surface ancillary data include pressure, temperature, and emissivity. Atmospheric ancillary data include temperature and water vapor profiles. Geometrical factors including solar and satellite zenith angles are also categorized as required ancillary inputs.

2.2. Radiative Transfer Modeling

The most critical single component of the retrieval algorithm is the forward radiative transfer model, i.e. the model which calculates the MOPITT signals given a particular atmospheric state, surface characteristics, and solar illumination and satellite viewing geometries. Since the forward model is integrated into the retrieval algorithm, and may be called many times during a retrieval for just a single pixel, the model must be both accurate and computationally efficient. A fast radiative transfer model known as 'MOPFAS' was developed specifically to accurately and efficiently calculate MOPITT radiances for both the CO and methane radiances and is the model incorporated into the retrieval algorithm described here.[6] The model is also used in the retrieval simulations to produce simulated MOPITT data which are fed to the retrieval algorithm.

2.3. Maximum Likelihood Inversion

The development of the retrieval algorithm follows the maximum likelihood inversion technique described by Rodgers[5] where, in the case of methane retrievals, both the measurement and the retrieved quantity (methane total column) are scalar quantities. Unlike the MOPITT carbon monoxide-channel radiances, the methane-channel radiances do not contain sufficient information to derive the methane vertical distribution (i.e. the methane vertical profile) but rather are well-suited to deriving the total amount of methane in a vertical column.

2.3.1. Methane radiance ratio

In the methane 2.2 micron band, thermal emission from the Earth's surface and atmosphere is generally negligible compared to reflected solar radiation. Thus, retrievals of methane are only feasible when the instrument faces the sunlit side of the earth. Both S_A and S_D are proportional to the intensity of solar radiation attenuated by absorption during two paths through the atmosphere in addition to a single surface reflection. Generally, the degree of atmospheric attenuation corresponding to S_A and S_D will differ greatly because of the much higher sensitivity of S_D to atmospheric methane. However, assuming that the surface reflectivity is independent of wavelength over the spectral width of the MOPITT methane bandpass filter, both S_A and S_D will be identically attenuated by surface reflectivity. Under this assumption, the ratio of S_D and S_A should be independent of surface reflectivity and therefore provide a more direct quantity from which to retrieve atmospheric methane

than either S_A or S_D individually. In addition, to the extent that the solar spectrum is independent of wavelength in the methane 2.2 micron band, the ratio of S_D and S_A should also be insensitive to fluctuations in solar intensity. For these reasons, the ratio

$$R \equiv S_D / S_A \tag{1}$$

is used as the measured quantity from which to retrieve methane total column. Throughout the rest of this paper, R^{OBS} refers to the ratio of the observed (measured) S_D and S_A values whereas R^T refers to the ratio of theoretical S_D and S_A values (as calculated by MOPFAS).

2.3.2. Weighting function calculation

The maximum likelihood technique requires derivatives of the theoretical radiance ratio (R^T) with respect to the retrieved quantity x (methane total column). These derivatives are known as weighting functions and are generally expressed in matrix form. In this case, however, where both the retrieval parameter (R) and retrieved quantity (x) are both scalar entities, the weighting function is also scalar. Therefore, the methane total column weighting function k is simply defined as

$$k \equiv dR^T / dx \tag{2}$$

Operationally, the weighting function k is calculated numerically according to Eq. (2) by scaling a given methane profile by some constant (near unity) and evaluating the corresponding changes in R^T (after running MOPFAS for the scaled profile) and x and then evaluating the ratio.

2.3.3 Iterative retrieval formula

Following Rodgers,[5] the iterative formula for generating the $(n+1)$st maximum likelihood estimate of the methane total column (x_{n+1}) from the nth estimate (x_n) is

$$x_{n+1} = x_0 + \left(\frac{c_x k_n}{c_x k_n^2 + c_R} \right) \left(R^{OBS} - R^T(x_n) - k_n (x_0 - x_n) \right) \tag{3}$$

where x_0 is the a priori methane total column, c_x is the a priori variance of methane total column, k_n is the weighting function evaluated at x_n, c_R is the signal variance (representing various sources of errors in the measured radiances), R^{OBS} is the observed ratio (S_D/S_A) signal, and $R^T(x_n)$ is the theoretical ratio signal evaluated at x_n.

Methane retrievals proceed iteratively in the following manner. For the initial guess methane profile, the initial guess methane total column x_0 is calculated. MOPFAS is then run to obtain $R^T(x_0)$. The weighting function k_0 is then calculated, as described previously. With fixed values for c_x and c_R, the first-guess methane total column x_1 is then calculated according to Eq. (3). To obtain the new methane profile corresponding to x_1, the initial guess methane profile is simply scaled by the ratio of the new estimate of x (x_1) to the previous estimate (x_0). The process is repeated to obtain successively more accurate estimates of x. After each iteration, a test is performed to check for algorithm convergence. Iterations cease when x changes by less than 0.2% in consecutive iterations. In simulations, the algorithm typically converges in two or three iterations.

A byproduct of the maximum likelihood technique is the retrieval error variance c_x^{rtv}, which indicates the uncertainty in the retrieved value of x. It can be shown that

$$c_x^{rtv} = \left(c_x^{-1} + \frac{k^2}{c_R} \right)^{-1} \tag{4}$$

3. NUMERICAL RETRIEVAL SIMULATIONS

Before conducting retrieval simulations, estimates of the a priori (methane profile and total column variance c_x) and signal variance c_R must be developed.

3.1 A Priori

A database of 525 in-situ methane profiles sampled from aircraft during 8 field campaigns and at 2 fixed sites representing a wide variety of tropical and mid-latitude atmospheric conditions over ocean and land were used both to produce the a priori and in retrieval simulations. In-situ methane data were supplemented with chemistry-model output for middle- and upper-atmosphere methane concentrations. All profiles were interpolated to a common pressure grid of 32 levels between 1000 and 0.1 mb and were numerically integrated to produce methane total column values. To maintain statistical independence between the profiles used to produce the a priori and the profiles used to conduct retrieval simulations, the set of 525 profiles was divided into two subsets. Each subset contains approximately the same number of profiles from each of the field campaigns which make up the superset. One subset was used exclusively as a 'training' set, (for the purpose of producing the a priori estimates) whereas the second set was used exclusively as a 'testing' set to assess the performance of the retrieval algorithm (see below). The training set profiles used to generate the a priori are plotted in Figure 1. The a priori methane profile was calculated as the mean profile of all profiles in the training set. The corresponding total column value for this profile was taken as x_0. The methane a priori total column variance c_x was taken to be the variance of the methane total column values over all profiles in the training set.

3.2. Radiance Error Sources

The sources of radiance error considered in this paper include instrumental noise (typically electronic noise) and forward model error. Generally, $S_A >> S_D$, whereas the statistical uncertainties of S_A and S_D are of similar magnitudes. Application of the chain rule to Equation 1 to obtain the instrumental ratio signal variance c_R^I then yields

$$c_R^I = c_D / S_A^2 \tag{5}$$

where c_D is the statistical variance of S_D and represents the estimated instrumental error in the measured difference signal . Within the retrieval simulations, c_D is taken to be a constant characteristic of the instrument and c_R^I is calculated using the input S_A value each time the retrieval algorithm is executed.

As described previously, the operational forward radiative transfer model MOPFAS was designed for both accuracy and computational efficiency, and therefore lacks the precision of a line-by-line model. MOPFAS is a parameterization of another radiative transfer model known as MOPABS, which is itself a derivative of the line-by-line radiative transfer model GENLN2.[6] The effect of forward model error as a source of retrieval error can be modeled in terms of a ratio signal variance term, analogous to the instrumental noise term c_R^I.[7] To estimate the ratio signal variance due to forward-model error c_R^{FME}, a statistical analysis was made of the radiance ratio errors between MOPFAS and MOPABS for all 263 training set profiles. For simulations in which both forward model error and instrumental error are included as sources of retrieval error, the total ratio signal variance c_R is simply taken as the sum of c_R^I and c_R^{FME}.

3. 3. Retrieval Simulation Procedure

Each methane profile in the test set, with corresponding temperature and water vapor profiles, was first run through MOPFAS to obtain 'true' values of S_D and S_A. To simulate the contaminating effects of the radiance errors described in the previous section, these values of S_D and S_A were then modified by adding 'noise' values using a random number generator which produced Gaussian-distributed noise values consistent with the estimated radiance ratio error c_R . These noise-contaminated radiance values were then fed to the retrieval algorithm along with the temperature and water vapor profiles from the true profile. After running the entire test set of methane profiles through this process, retrieved methane total column values for the two methane cells were averaged and retrieval statistics (e.g. root-mean-square total column error and root-mean-square fractional total column error) were calculated for the ensemble.

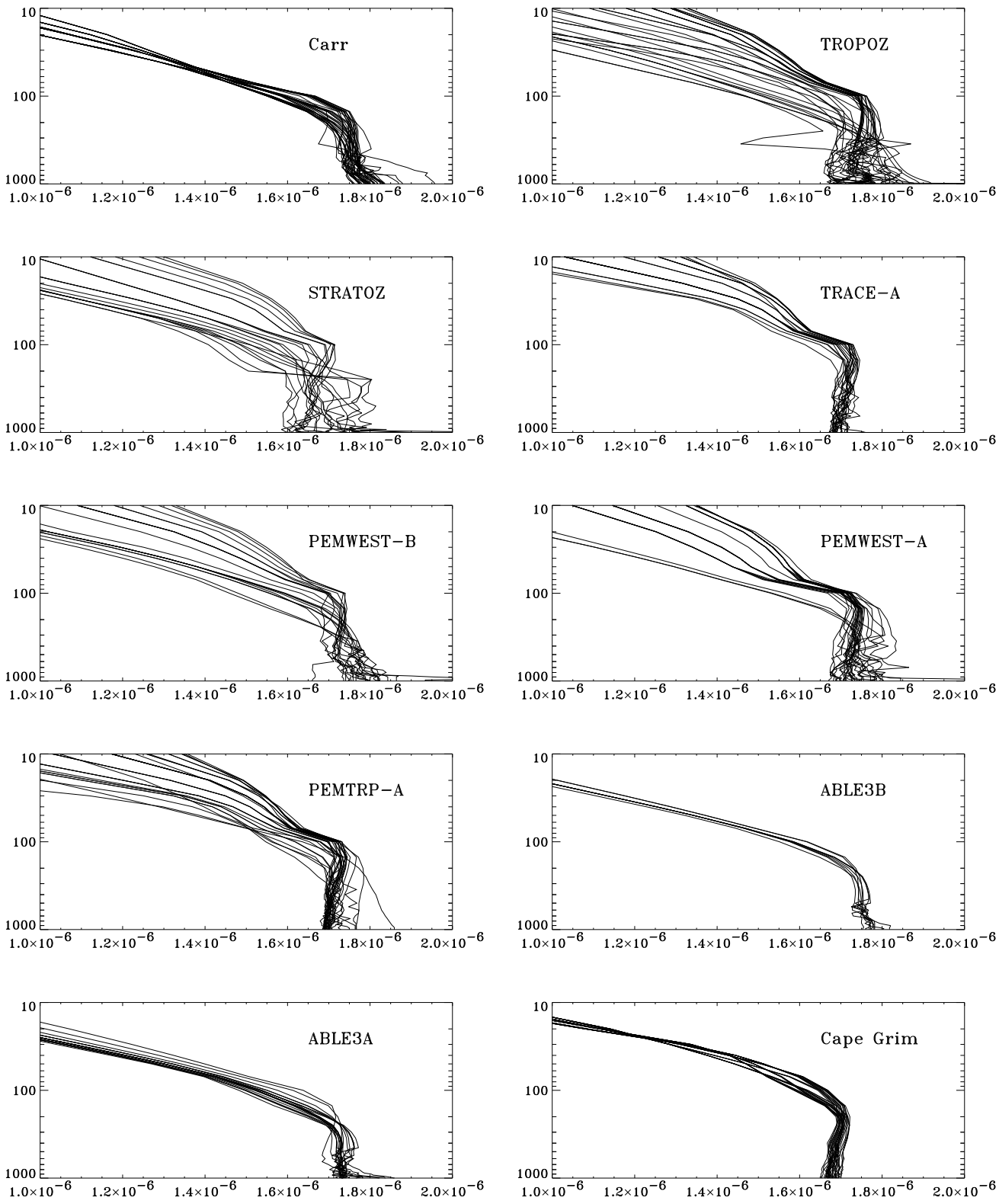

Figure 1. Training-set methane profiles accumulated during 10 field campaigns and used as basis of a priori. Horizontal axis in each figure is methane volume mixing ratio; vertical axis is pressure in millibars.

3.4. Simulation Results

Retrieval simulations were conducted to quantify the dependence of retrieval performance on radiance error source, solar zenith angle and surface reflectivity. Simulations were performed with two sets of radiance ratio errors c_R, corresponding to instrumental-noise only, and instrumental noise plus forward-model error. Each set of simulations was also performed with both high (R_{sfc} = 0.20) and low (R_{sfc} = 0.01) surface reflectivity values, which were chosen to represent land surfaces and open water, respectively.[8] Finally, simulations were performed at solar zenith angle Θ_{sol} values of 0 and 60 degrees. Retrieval simulation results are presented in Table I.

Table I. Retrieval simulation results for indicated combinations of solar zenith angle, surface reflectivity, and radiance error sources. Instrumental radiance error sources are indicated by 'Inst.', forward-model-error is indicated by 'FME.'

Θ_{sol} (degrees)	R_{sfc}	Simulated Radiance Error Sources	RMS CH_4 total column error (mol/cm^2)	RMS CH_4 total column fractional error
0	0.20	Inst.	5.62×10^{16}	0.00160
60	0.20	Inst.	8.81×10^{16}	0.00253
0	0.01	Inst.	6.15×10^{17}	0.01713
60	0.01	Inst.	7.09×10^{17}	0.01980
0	0.20	Inst., FME	5.33×10^{17}	0.01535
60	0.20	Inst., FME	4.98×10^{17}	0.01437
0	0.01	Inst., FME	6.50×10^{17}	0.01819
60	0.01	Inst., FME	7.11×10^{17}	0.01986

The simulation results for the cases of high surface reflectivity and no forward model error indicate very low retrieval errors (less than 0.3% rms total-column fractional error) for both solar zenith angle values. These retrieval error values indicate the performance of the retrieval algorithm as the result of 'fundamental' error sources including instrument noise and methane profile shape variability. Retrieval errors increase significantly (up to 1-2% fractional error) as the result of both low surface reflectivity and forward model error. Retrieval degradation due to low surface reflectivity might be partially offset by pixel-level signal averaging (with corresponding degradation in spatial resolution). Likewise, refinements in MOPFAS will be needed in order to reduce the contribution of forward model errors to the ultimate retrieval error.

3.5. Retrieval diagnostics: Averaging Kernel

In order to compare retrieval results against either in-situ measurements or other remote-sensing retrievals, the averaging kernel must be specified. The averaging kernel quantifies the degree to which the retrieved quantity depends (differentially) on the true quantity. For the methane retrievals described here, the averaging kernel describes the dependence of the retrieved methane total column on the true methane profile. To evaluate the averaging kernel, we chose to use the perturbative approach of Pougatchev.[9] Specifically, retrievals were simulated for a series of methane profiles, each of which was 'perturbed' at a different atmospheric level. The magnitude of the perturbation was chosen to simultaneously optimize linearity (which favors small perturbations) and numerical precision (which favors large perturbations). Perturbation of the initial profile results in changes to both the true methane total column and retrieved methane total column. The averaging kernel value at a specific level is simply the ratio of the resulting change in the retrieved methane total column value to the corresponding change in the true value. Thus, if the a priori methane profile is used as the baseline 'unperturbed' profile, the averaging kernel value for level k A^k is simply

$$A^k = \frac{(x_{rtv}^k - x_0)}{(x_{true}^k - x_0)} \tag{6}$$

where $x_{rtv}{}^k$ is the retrieved methane total column for the profile perturbed at level k, and $x_{true}{}^k$ is the corresponding true methane total column value. Total column methane averaging kernels determined this way for a surface reflectivity value of 0.20, no forward model error, and solar zenith angles of 0 and 60 degrees are shown in Fig. 2.

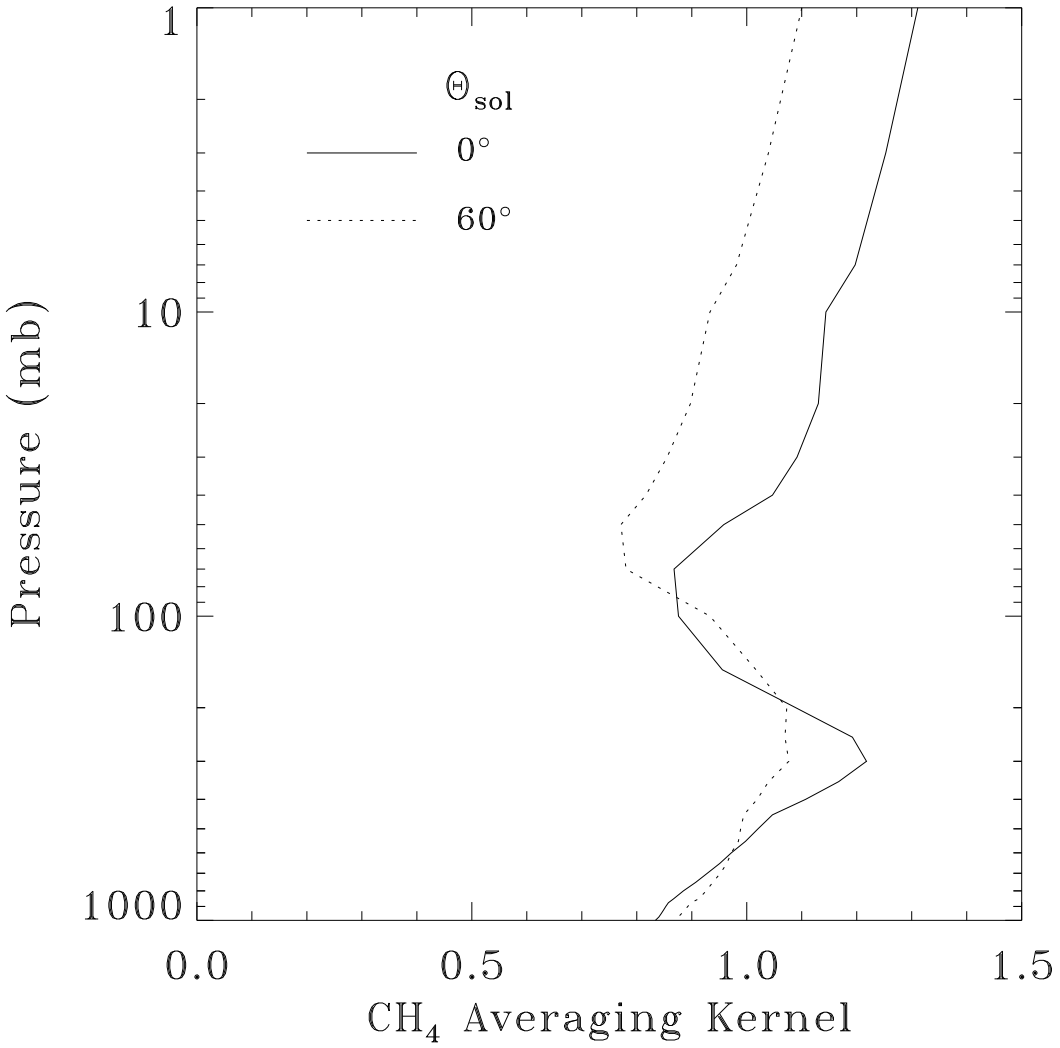

Figure 2. Methane total column averaging kernel for surface reflectivity of 0.20, no forward model error, and solar zenith angles of 0 and 60 degrees.

4. SUMMARY

The current implementation of the methane total column retrieval algorithm for MOPITT has been described. The algorithm incorporates the principle of maximum likelihood. The ratio of MOPITT's methane-channel 'Difference' and 'Average' signals is used as the measured quantity from which the methane total column is retrieved. A scaling factor applied to the a priori methane profile is adjusted according to the measured ratio signal and its uncertainty, the a priori value of methane total column, and the theoretical derivative of the ratio signal with respect to methane total column (i.e. the weighting function).

Retrieval simulations using an independent set of in-situ methane profiles were performed to estimate the retrieval algorithm's sensitivity to various sources of retrieval error. For surface reflectivity values typical of land, fundamental sources of retrieval error including instrument noise and methane profile shape variability produce methane column retrieval errors less than 0.3%. Retrieval errors between 1 and 2% are observed for simulations for low reflectivity surfaces (typical

of open water) and for simulations which include the effects of forward model error. Methods for reducing these sources of error, such as pixel-level signal averaging, are being explored.

ACKNOWLEDGMENTS

The NCAR MOPITT project is supported by the National Aeronautics and Space Administration (NASA) Earth Observing System (EOS) program. The National Center for Atmospheric Research (NCAR) is supported by the National Science Foundation.

REFERENCES

1. H. Rodhe, "A comparison of the contribution of various gases to the greenhouse effect," *Science* **248**, 1217-1219, 1990.
2. E. J. Dlugonecky, K. A. Masaire, P. M. Lang, et al, "A dramatic decrease in the growth rate of atmospheric methane in the northern hemisphere during 1992," *Geophysical Res. Lett.*, **21**, pp. 45-48, 1994.
3. J. R. Drummond, G. P. Brasseur, G. R. Davis, J. C. Gille, J. C. McConnell, G. D. Pesket, H. G. Reichle, and N. Roulet, "MOPITT Mission Description Document (MDD)," available from Dept. of Physics, University of Toronto, Toronto, ON, M5S 1A7, Canada
4. Mark W. Smith, "Method and results for optimizing the MOPITT methane bandpass," *Appl. Opt*. **36**, pp. 4285-4291, 1997.
5. C. D. Rodgers, "Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation," *Reviews of Geophys. and Space Phys*. **14**, pp 609-624, 1976.
6. D. P. Edwards, C. Halvorson, and J. C. Gille, "Radiative transfer modeling for the EOS Terra satellite Measurement of Pollution in the Troposphere (MOPITT) instrument," in press, *J. Geophys. Res*.
7. Crispin J. Marks and Clive D. Rodgers, "A retrieval method for atmospheric composition from limb emission measurements," *J. Geophys. Res.* **98**, pp. 14939-14953, 1993.
8. Zhen Z. Yu and J. R. Drummond, "A global surface reflectivity data set for the 2.2-2.35 μm region," *Intl. J. Remote Sensing*. **19**, p. 331, 1998.
9. N. Pougatchev, personal communication.