The EOS MOPITT experiment:

Extracting the information from the measurements

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ABSTRACT

This paper will serve as an overview of the challenges to the recovery of information on atmospheric CO and CH_4 from the measurements made by the MOPITT instrument that has been described by Drummond et al.[1]. It will also provide a context and introduction to several of the following papers that go into greater detail on particular topics, and outline plans for the data processing. Here we briefly outline the principles of correlation radiometry as used by MOPITT, and introduce the principles behind the retrievals. After noting plans for data processing, we discuss our approach to data validation, and the ability to see global distributions of CO in the MOPITT data.

1. INTRODUCTION

The Measurement Of Pollution In The Troposphere (MOPITT) instrument measures the upwelling radiation from the earth's surface and atmosphere in the regions of the carbon monoxide (CO) fundamental at 4.6 µm, and its first overtone band at 2.3 µm, and the region of a methane (CH_4) band at 2.3 µm. The radiation in the longer wavelength region is dominated by thermal emission, with a small component due to reflected solar radiation while the radiation at 2.3 µm is completely due to reflected solar radiation. However, in both of these regions there is strong interference by spectral lines of other atmospheric gases, especially water vapor, but also nitrous oxide (N_2O) and ozone (O_3). In order to reduce the effects of this interference, MOPITT makes use of correlation radiometry. In this technique the signal from the atmosphere is measured through a cell of the target gas (CO or CH_4). By modulating the amount of gas in the cell, either by varying the pressure or the length, corresponding changes are induced in the transmission of the cell, and thus in the measured. With more absorbing gas in the cell, the transmittance of the signal will be smaller than when there is less gas in the cell. MOPITT combines these signals into an Average and a Difference signal. The transmittance of the Average signal is near unity for all frequencies except at the positions of the lines of the target gas, where it dips to smaller values. By contrast, the transmittance of the Difference signal is near zero everywhere except at the positions of the target gas lines, where its response increases[2]. It follows that the Average signals will be responsive to the surface and interfering gases, while the Difference signals will be more responsive to the target gas in the atmosphere.

The spectral character of the signal modulation depends on the mean pressure in the cell. At higher cell pressures, the modulation takes place in the wings of the spectral lines, which in the atmosphere are formed at higher pressures and lower altitudes. Conversely, at lower cell pressures, the modulation takes place near the centers of the lines, which are formed at lower pressures, higher in the troposphere. MOPITT has 4 cells operating at 4.6 µm, with mean pressures between 38 and 800 mbar, resulting in peak contributions to the Difference signals ranging from the lower to the upper troposphere[3]. It should be noted that, for the 4.6-µm (thermal) channels, the signal depends on the temperature contrast between the surface and the lowest layer of the atmosphere. In the usual condition when these temperatures are similar, there is no contribution from the surface layer, which therefore ordinarily can't be seen in these channels.

By contrast, the signals in the 2.3 µm (solar) channels are affected by absorption at all levels. There are large variations in both the Average and Difference signals in these channels, because of the large variations of the albedo of the land surface or

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clouds. Consequently, the ratio of the Difference to Average signal is used as a variable; the maximum contribution to this ratio comes from the lowest atmospheric layer, thus complementing the thermal channels[3].

2. RETRIEVAL PRINCIPLES

In order to retrieve the CO and CH4 distributions, we must be able to calculate signals from the atmosphere for different amounts of the target gas. The Average or Difference signals may be calculated from the expression

$$S^{A,D} = \int_{\Delta\nu} \{ I_\nu(sfc)d\nu + \int_{\tau_{sfc}}^{1} (B_\nu(\tau) - I_\nu(sfc))d\tau \} R_\nu^{A,D} d\nu$$

Where S is the received signal, superscripts A and D refer to the Average and Difference values, I_ν is the radiance at frequency ν, sfc refers to surface conditions, B is the Planck black body function, τ is the monochromatic optical depth, and R the instrumental spectral response.

Operational evaluation of this expression requires several things. First, there must be an accurate and fast scheme to calculate the outgoing radiances, the Forward Radiance Model. Francis et al.[4] describe the model that MOPITT will use. R must be determined during the test and calibration phase of the instrument fabrication. Mond et al.[5, 6] describe some of the laboratory measurements that have been made to test and characterize MOPITT. Finally, vertical distributions of temperature and water vapor must be available for the for the time and location for which calculations are made. For these, MOPITT plans to use the products of the Data Assimilation Office at NASA's Goddard Space Flight Center. These have the advantage of a detailed surface energy balance model, which is expected to provide good estimates of surface temperature as well as the atmospheric quantities. In addition, the climatological distributions of fixed gases (e.g. N_2O) are needed. Finally, a value of surface reflectivity or emissivity is needed, since, if ε is the emissivity

$$I_\nu(sfc) = B_\nu(sfc)\varepsilon_\nu + I_\nu(sfc)(1 - \varepsilon_\nu)$$

For the retrieval itself, MOPITT will make use of the maximum likelihood method (Rodgers[7, 8]). This may be outlined briefly by noting that

$$\mathbf{S} = \mathbf{F}(\mu, b) + N_e$$

$$= \mathbf{F}(\mu^0, b) + \mathbf{K}(\mu - \mu^0) + N_e$$

where F (μ,b) is the forward model, which depends on the CO mixing ratio μ and other parameters b, and n_e is the measurement noise. μ^0 is a linearization point, hopefully not too far from the correct answer, and the weighting function is given by

$$K^{A,D}_{i,j} = \partial S^{A,D}_{i} / \partial \mu_{j}.$$

In addition, there is a priori information on the CO distribution, μ_a, and a measure of its uncertainty, its covariance matrix C_a. These may be regarded as a virtual measurement and its uncertainty. The maximum likelihood method combines the measurement with the virtual measurement, weighting each by the inverse of its uncertainty, to lead to the result

$$\hat{\mu} = \left(\mathbf{C}_\alpha^{-1} + \mathbf{K}^T \mathbf{C}_\varepsilon^{-1} \mathbf{K}\right)^{-1} \left(\mathbf{C}_\alpha^{-1} \mu_\alpha + \mathbf{K}^T \mathbf{C}_e^{-1} \mathbf{S}\right)$$

with covariance

$$\hat{\mathbf{C}} = \left(\mathbf{C}_\alpha^{-1} + \mathbf{K}^T C_e^{-1} K\right)^{-1}$$

Wang et al.[9] and Deeter et al.[10] describe the application of this approach to synthesized MOPITT CO and methane data, respectively.

The discussion to this point has been limited to clear, cloud-free conditions. Unfortunately for tropospheric retrievals, this is not always the case. It has been estimated that the MOPITT pixels, 22 x 22-km in size, will be cloud free only about 25% of the time. The rest of the time they will be characterized either by broken clouds, or a solid undercast. The challenges to the MOPITT data processing are to detect clear sky cases, and, where possible, to remove the effects of clouds from the radiances, to allow the retrieval to proceed. Warner et al.[11] outline methods for detecting clear sky cases, using threshold and other methods, while Ziskin et al.[12] describe tests of these algorithms using MODIS Airborne Simulator (MAS) measurements.

The initial stages of the retrieval bring together the radiance signals, the ancillary meteorological data, and a first approximation to the CO distribution to do calculations that are required by the threshold method in the cloud detection. Pixels determined to be clear proceed to the inversion stage, while others are checked to see whether the radiances can be "cloud cleared"; if this is successful, they are also sent to the inversion stage. The inversion is iterated, to get around any non-linear effects of starting the inversion too far from the final result.

3. DATA PROCESSING

The standard MOPITT scientific data products are:

- Level 1-Calibrated and geo-located radiances
- Level 2-Geolocated geophysical data
    - Tropospheric CO profiles. This will be the mixing ratio at 7 levels
    - Total CO columns
    - Total CH_4 columns
- Level 3-(experimental at launch)
    - Gridded global CO distributions on 7 levels
    - Gridded CO columns
    - Gridded CH_4 columns

The data will be processed at the National Center for Atmospheric Research, in a Science Investigator-led Processing System (SIPS) for the first 18months after launch. Processing after this will nominally be at the Langley Distributed Archive and Analysis Center (LDAAC), but this is expected to depend on subsequent algorithm developments
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The MOPITT measurement data (Level 0 or L0) will flow from the Terra spacecraft to LDAAC, and on to the MOPITT SIPS. Here it will be ingested, catalogued, and sent to the L0-L1 Processor, in which the raw counts from the instrument are converted to calibrated, geolocated radiances, with associated quality flags. The results will be catalogued, and a copy sent back to the LDAAC for distribution to users. The data will also be sent to the L1-L2 Processor, for retrieval into CO profiles, with quality flags, metadata and browse products. Again, the output will be catalogued and sent back to the LDAAC, and also to the L2-L3 Processor for gridding. At all levels the quality flags will be reviewed to ensure that the data are being processed to completion and that convergence criteria are met. In addition, the products will be visually inspected to ensure the reasonableness of the data. At the conclusion of these steps, quality flags will be set to indicate to users the confidence they can have in the products.

4. DATA VALIDATION

MOPITT is the first instrument to measure signals from the troposphere with Pressure Modulator Cells and Length Modulator Cells, so validation of its results will be very important. It will not be straightforward, as there are very few operational measurements of tropospheric CO. Much of the initial validation will be through the careful verification of the precision and accuracy of the radiometry, coupled with pre-flight testing of the retrieval algorithms and their sensitivity to various instrumental and external factors.

After launch the MOPITT approach is to concentrate attention on the simplest cases first, to ensure that those are understood, before focussing on the more difficult cases. Therefore initial attention will go to cloud-free cases.

4.1 Cloud-free situations

These cases are clearly simpler than those with clouds are. Initial efforts will focus on oceanic cases during daytime, since clouds should be easily detected against the dark background of the ocean at 2.3 μm. In addition, the surface of the ocean has a stable and reasonably uniform sea surface temperature (SST). Initial checks will be made to ensure that the S^A's lead to correct values for the SST, and that the S^D's are consistent with expected values of the CO distribution. When these tests are successfully passed, retrievals will be carried out, and compared with a priori values. Finally, comparisons will be made with coincident measurements.

While detection of clouds over the ocean in darkness will be more difficult, the use of thermal channel thresholds will be checked during daytime. These will then be used at night to find cloud-free conditions, and the same checks as the daytime checks will be done for night conditions.

Effort then will move on to cloud-free conditions over land, where the underlying albedo is higher and more variable in space and time. The procedures will follow the same sort of logic as over the ocean.

4.2 Broken-cloud situations

Initially the easiest place to test this will be over the oceans in daylight, because of the uniform underlying surface. Again, this will be extended to nighttime conditions, building on the daytime experience. Subsequently this will be extended to the land surface, using the lessons learned over the oceans.

4.3 Measurements for MOPITT validation

Several types of coincident measurements will be made to validate the MOPITT results. Most direct are the aircraft measurements of CO profiles by in-situ samplers by Novelli et al.[13] at Hawaii and Samoa over the ocean, and at Carr, Colorado, Boston Massachusetts, and Barrow, Alaska over land.

Two airborne correlation radiometers that simulate MOPITT operation will also be used to validate MOPITT results. These are the MOPITT Airborne Test Radiometer, described by Smith et al.[14], and MOPITT-A, an instrument that will be very similar to MOPITT and designed for flights on the ER-2 (Bailak et al.[15]).
Ground based spectroscopy from about a dozen sites covering a wide range of latitudes will also be used to measure total columns, with perhaps a very crude representation of the vertical variation. These are discussed by McKernan[16] and Tolton[17].

GLOBAL DATA

Model simulations for a typical October show strong CO plumes in the upper troposphere from regions of biomass burning in South America and South Africa. Near the equator these are advected westward by the prevailing winds. In southern mid-latitudes, however, the plumes become entrained by the westerlies, resulting in the transport of CO for thousands of kilometers across the Indian Ocean. Initial simulations of MOPITT results, including the effects of instrument noise, but not of clouds, indicate that this long-range transport should be readily seen. These data will provide enormous new insights into the transport and chemical transformations of CO in the troposphere, and thus the first detailed insight into the chemistry of the global troposphere.

SUMMARY

A retrieval algorithm based on optimal estimation has been developed to retrieve atmospheric CO profiles and columns, and CH4 columns from MOPITT data and ancillary meteorological information. Simulations based on realistic profiles show that the requirements for 10% precision in the CO profiles are attainable. The data will be processed initially at NCAR. A comprehensive data validation plan is in place. A pre-launch validation exercise has been conducted to compare different correlative measurements. The MOPITT results will show the significant dynamical and chemical processes affecting global CO and CH_4.

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REFERENCES

1. J. R. Drummond, P. L. Bailey, G. Brasseur, G. R. Davis, J. C. Gille, G.D. Peskett, H. K. Reichle, Jr., N. Roulet, G. S. Mand, and J. C. McConnell, Early mission planning for the MOPITT instrument (*Invited Paper*), *Optical Spectroscopic Techniques and Instrumentation forAtmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
2. J. R. Drummond, Measurements of Pollution in the Troposphere (MOPITT), in the *Use of EOS for Studies of Atmospheric Physics*, edited by J. C. Gille and G. Visconti, pp. 77-101, North-Holland, New York, 1992.
3. L. Pan, D. P. Edwards, J. C. Gille, M. Smith, and J. Drummond, Satellite remote sensing of tropospheric CO and CH_4: Forward model studies of the MOPITT instrument, *Appl. Opt*., 34 pp. 6976-6988, 1995.
4. G. L. Francis, D. P. Edwards, and J. C. Gille, Channel radiance calculations for MOPITT forward modeling and operational retrievals, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, *SPIE Proceedings*, Vol. 3756, 1999 (this issue).
5. G. S. Mand, G. V. Bailak, Z. Z. Yu, B. T. Tolton, E. McKernan, and J. R. Drummond, Preflight testing of the MOPITT instrument, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
6. G. S. Mand, Z. Z. Yu, B. T. Tolton, N. Mak, and J. R. Drummond, Early look at real MOPITT data, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
7. C. D. Rodgers, Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation, *Rev. Geophys*., 14, 609-624, 1976.
8. C.D. Rodgers, Characterization and error analysis of profiles retrieved from remote sounding measurements, *J. Geophys. Res*., 95, 5587-5595, 1990.
9. J. Wang, M. N. Deeter, J. C. Gille, and P. L. Bailey, Retrieval of tropospheric carbon monoxide profiles from MOPITT measurements: algorithm description and simulations, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
10. M. N. Deeter, J. Wang, J. C. Gille, and P. L. Bailey, Retrieval of tropospheric methane from MOPITT measurements: algorithm description and simulations, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
11. J. Warner, J. C. Gille, D. P. Edwards, and P. L. Bailey, Cloud detection and clearing from the MOPITT instrument, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
12. D. Ziskin, J. Warner, P. L. Bailey, and J. C. Gille, Validating MOPITT Cloud Detection Techniques with MAS Images, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
13. P. C. Novelli, A. A. Masarie, P. Tans, and P. M. Lang, Recent changes in atmospheric carbon monoxide in the troposphere, *J. Geophys*. Res., 97, 20,731-20,750, 1992.
14. M. W. Smith, S. R. Shertz, and N. Delen, MOPITT airborne test radiometer (MATR): an instrument for remote sensing of atmospheric carbon monoxide, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
15. J. R. Drummond, G. V. Bailak, G. R. Davis, L. Jounot, G. S. Mand, A. Phillips, and B. T. Tolton, MOPITT airborne validation instrument: MOPITT-A, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).

16. E. McKernan, B. T. Tolton, J. R. Drummond, and L. Yurganov, MOPITT validation using ground-based IR spectroscopy, *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).
17. B. T. Tolton, L. Yurganov, E. McKernan, A. Predoi-Cross, and E. T. Grechko, Intercalibration of medium-resolution grating spectrometers for MOPITT validation, *Optical Spectroscopic Techn0iques and Instrumentation for Atmospheric and Space Research III*, SPIE Proceedings, Vol. 3756, 1999 (this issue).