Channel radiance calculations for MOPITT forward modeling and operational retrievals

G.L. Francis, D.P. Edwards, and J.C. Gille

Atmospheric Chemistry Division
National Center for Atmospheric Research*

ABSTRACT

The MOPITT (Measurement of Pollution in the Troposphere) instrument, to be launched on the Earth Observing System Terra platform, employs gas-correlation spectroscopy to measure profiles of tropospheric carbon monoxide and the total column of methane. The modeling of the instrument, and the associated radiative transfer, comprise the forward model employed in the retrieval calculations. The MOPITT forward model has been implemented through a hierarchy of radiation codes whose salient features are reviewed here.

Keywords: forward modeling, correlation spectroscopy, MOPITT, carbon monoxide, methane

1. INTRODUCTION

The MOPITT instrument, to be launched on the EOS Terra platform, will provide the first extended global measurements of tropospheric carbon monoxide and methane. Profiles of CO will be determined at several levels in the troposphere, as well as CO and CH_4 column abundances. The CO profile and total column will have an anticipated accuracy of 10 percent, with the CH_4 column determined to 1 percent.

There is considerable interest in extended global measurements of CO and CH_4. CO exhibits seasonal and regional variations due to industrial and agricultural processes, particularly biomass burning. It also plays a role in HO_x chemistry, influencing the distribution of the hydroxyl radical OH, a major oxidizing component of the troposphere. Due to its fairly long lifetime, CO can be used as an atmospheric tracer of three-dimensional tropospheric motion. The vertical CO distribution can mirror chemical transport by deep convection, which contributes to troposphere-stratosphere exchange through convective overshoots at the tropopause. The global distributions

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of CO and CH_4 column abundance can provide vertically-averaged signatures of organized motion by tropospheric wave activity. Both CO and CH_4 chemically influence the tropospheric O_3 distribution. CH_4 is also increasing in the atmosphere and the anthropogenic sources of this increase are not well identified. In the stratosphere, this increase is implicated in observed increases in water vapor through CH_4 oxidation.

MOPITT employs gas correlation radiometers to extract a target gas signal and separate its contribution to the top-of-atmosphere (TOA) radiance from that due to contaminating species and the underlying surface. Both pressure-modulated radiometers (PMR) and length-modulated radiometers (LMR) are employed[1]. In a gas correlation radiometer, TOA radiance passes through a cell containing the same gas as the target gas being measured. For MOPITT the target gas is either CO or CH_4, depending on the channel. By regularly varying the cell length (LMR) or the cell pressure (PMR) between two states, the optical depth of each correlation cell is modulated at the positions of the spectral lines of the target gas. As a result, two different signals are obtained in each channel, corresponding to each of the two cell states. The average (A) of these two signals yields information about the surface and contaminating gases, while the difference (D) of the two signals gives information about the target gases. Since radiative processes in the line wings occur at lower altitudes, a set of appropriate PMR and LMR channels can sample radiance originating at different altitudes, thereby providing profile information.

Forward modeling of the satellite channel radiances must combine accuracy and precision while providing for variations in target and contaminating gases, temperature, viewing geometry and surface properties. To achieve this, a set of radiation models has been developed and applied to the calculation of channel radiances for the MOPITT instrument. Within their range of applicability, each in turn is an effective tool.

In the following sections we briefly review the salient features of these models and discuss their structure and application.

2. THE MOPITT EQUATION OF TRANSFER

The i-th channel radiance measured by MOPITT has the form

$$S_i^{A,D} = \int I(\nu) h_i^{A,D}(\nu) w_i(\nu) d\nu \tag{1}$$

where $S_i^{A,D}$ is the average or difference channel radiance, $h_i^{A,D}(\nu)$ is the correlation cell A or D response, and $w_i(\nu)$ is the i-th normalized channel blocker filter. Assuming clear-sky conditions, no scattering and an underlying Lambertian surface, the TOA monochromatic radiance $I(\nu)$ has the following form:

$$
\begin{aligned}
I(\nu) = & \int_{p_s}^{0} B(\nu, T) d\tau(\nu, p, \theta_{sat}) \\
& + \ \epsilon(\nu) B(\nu, T_s) \tau(\nu, p_s, \theta_{sat}) \\
& + \ (1 - \epsilon(\nu)) \frac{F_d(\nu)}{\pi} \tau(\nu, p_s, \theta_{sat}) \\
& + \ (1 - \epsilon(\nu)) \frac{F_\odot(\nu)}{\pi \sec \theta_\odot} \tau(\nu, p_s, \theta_\odot) \tau(\nu, p_s, \theta_{sat})
\end{aligned} \tag{2}
$$

Here $B(\nu, T)$ is the Planck function at temperature T, $F_d(\nu)$ is the downward diffuse thermal flux at the surface, $F_\odot(\nu)$ is the solar flux at TOA, $\epsilon(\nu)$ is the surface emissivity and $\tau(\nu, p, \theta)$ is the monochromatic transmittance from pressure level p to TOA at angle θ. T_s and p_s denote surface temperature and pressure, respectively. Depending on the particular channel, one or more of the terms appearing here are dominant. In the CO thermal band ($2110 - 2230\ cm^{-1}$) the TOA radiance is dominated by surface emission as well as atmospheric absorption and emission. These are the first two terms on the right hand side of Equation (2). In both the CO shortwave band ($4220 - 4340\ cm^{-1}$) and the CH_4 shortwave band ($4280 - 4600\ cm^{-1}$), the TOA radiance during the day is dominated by reflected solar radiation, the fourth term. Downwelling thermal radiation reflected by the surface is given by the third term, which makes a non-negligible contribution in the CO thermal band, especially for low surface temperatures.

Together, the instrument response characteristics (Equation 1) and the equation of transfer (Equation 2) comprise the forward model used by MOPITT. It provides the radiances seen by the instrument under the conditions of the measurement.

3. THE MOPITT FORWARD MODEL HIERARCHY

3.1 GENLN2: Line-by-line calculations

Gas correlation spectroscopy introduces a high resolution spectral filter into the measurement process, having line widths of order 0.1 cm^{-1}. In addition, calculations with spectral resolutions as fine as 0.0025 cm^{-1} are required to construct the databases which are key components of the higher-level MOPITT radiation codes MOPABS and MOPFAS discussed below. Line-by-line (LBL) calculations must therefore be performed to provide these filters and databases. These are provided by the general purpose radiance and transmittance model GENLN2[2]. GENLN2 incorporates Voigt line shapes throughout, with full treatment of line wings, the effect of overlapping spectral lines both within the same band and between bands, and continuum absorption. It uses the HITRAN96 database and performs optimal atmospheric layering as well as ray tracing in spherical geometry, and a two-stage spectral calculation for regions close to, and far from, line center.

Although too cumbersome for operational use, TOA radiances provided by GENLN2 give benchmarks against which faster MOPITT codes can be assessed. GENLN2 LBL calculations have previously been applied to many other satellite instruments, and are currently in use for the development[3] of the HIRDLS[5] (High Resolution Dynamics Limb Sounder) instrument scheduled for launch aboard EOS-CHEM.

3.2 MOPABS: An optical-depth lookup table model

An intermediate step in the MOPITT radiation code hierarchy, MOPABS[4] computes channel radiances through a monochromatic absorption coefficient fitting scheme. This technique explicitly mirrors much of the underlying physics of the radiative transfer, permitting the calculation to be readily adapted for use by other instruments. In particular, the MOPABS method is being applied to model radiances for the MOPITT Airborne Test Radiometer (MATR) and the MODIS (Moderate Resolution Imaging Spectrometer) Airborne Simulator (MAS). Radiances from the latter are being used to develop cloud-clearing algorithms for use in MOPITT retrievals.

The essence of the MOPABS algorithm can be summarized as follows. LBL calculations are performed with GENLN2, giving monochromatic optical depths $\Delta K_l^{g,ref}(T_l^{ref})$ for each gas g and each layer l in an appropriate reference atmosphere having specified temperature T_l^{ref} and constituent column abundances $\Delta A_l^{g,ref}$ $(l = 1, n)$. A similar calculation is performed for the same atmosphere with layer temperatures artificially changed to $T_l^{ref} \pm 50\ K$. A quadratic polynomial fit of the logarithm of the optical depth against temperature is then made in each layer over this temperature range, giving frequency-dependent quadratic coefficients $\{a_l, b_l, c_l\}$. To this point all quantities are pre-computed.

Two steps are required to obtain monochromatic optical depths for a given test atmosphere at run-time. Denote the test atmosphere temperatures in layer l by T_l, and the corresponding layer column abundances for gas g by ΔA_l^g $(l = 1, n)$. In the first step, the optical depth for gas g at temperature T_l in the presence of the *reference* constituents follows from the quadratic fit as

$$\Delta K_l^{g,ref}(T_l) = \exp(a_l + b_l(T_l - T_l^{ref}) + c_l(T_l - T_l^{ref})^2).$$

In the second step, the monochromatic optical depth in layer l of the test atmosphere for gas g is obtained by a rescaling:

$$\Delta K_l^g(T_l) = \Delta K_l^{g,ref}(T_l)\frac{\Delta A_l^g}{\Delta A_l^{g,ref}}.$$

Knowing $\Delta K_l^g(T_l)$ in each layer, the monochromatic transmittance from level p_l to TOA at zenith angle θ is obtained as follows:

$$\tau(\nu, p_l, \theta) = \exp\left[-\sum_{l'=l}^{1}\sum_{g}\Delta K_{l'}^g(T_{l'})/\sec\theta\right].$$

Then the TOA radiances follow from Equation 2 and the channel radiances from Equation 1.

This method has essentially line-by-line accuracy and is considerably faster. Channel radiance calculations for a given test atmosphere can typically be completed in a few minutes. While this is still too slow for operational retrievals, MOPABS is an important tool for the development of a truly fast forward model. In addition, MOPABS has broad applications to other MOPITT work, as mentioned earlier.

3.3 MOPFAS: The MOPITT operational fast forward model

The MOPFAS[4] code currently provides the fast forward model calculations used by MOPITT. It achieves faster performance than MOPABS by reformulating the calculation so that time-consuming spectral integrations are avoided. To accomplish this, Equations (1) and (2) are collectively regarded as a statement about spectrally integrated quantities, particularly spectrally integrated transmittances, or products thereof.

Specifically, we define the integrated, normalized channel transmittance from TOA to level p_l at angle θ for the channel response function $\phi_i^{A,D}(\nu)$ as

$$\mathcal{T}_i^{A,D}(p_l,\theta) \equiv \frac{1}{\Phi_i^{A,D}} \int_{\Delta\nu_i} \tau(\nu,p_l,\theta)\ \phi_i^{A,D}(\nu) d\nu$$

where

$$\Phi_i^{A,D} \equiv \int_{\Delta\nu_i} \phi_i^{A,D}(\nu) d\nu.$$

Each term in Equation (1) and (2) can then be written using $\mathcal{T}$ or products of $\mathcal{T}$. For example, the signal component due to atmospheric emission takes the form

$$S_i^{A,D}(\mathrm{AtmTh}) = \Phi_i^{A,D} \sum_{l=L}^{1} B_i(\overline{T}_l)[\mathcal{T}_i^{A,D}(p_{l-1},\theta_{\mathrm{sat}}) - \mathcal{T}_i^{A,D}(p_l,\theta_{\mathrm{sat}})]. \tag{3}$$

In Equation (3), $\overline{T}_l$ is the layer-mean temperature, θ_{sat} is the satellite zenith angle and we assume the spectral variation of the Planck function $B_i(\overline{T}_l)$ over the channel passband can be neglected. Similar expressions hold for the remaining three terms in Equation (2).

It is useful to define an effective absorption coefficient $\overline{k}_l^g(\theta)$ in each pressure layer l for each gas g,

$$\overline{k}_l^g(\theta) \equiv \frac{-1}{\Delta A_l^g(\theta)} \ln\left[\frac{\mathcal{T}^g(p_l,\theta)}{\mathcal{T}^g(p_{l-1},\theta)}\right] \tag{4}$$

which determines $\mathcal{T}$ recursively. In this way, the problem of computing channel radiances is reduced to determining $\overline{k}_l^g(\theta)$.

The OPTRAN[7,8] regression scheme is applied to establish a correspondence between $\overline{k}$ and atmospheric state profiles, such that the former can be inferred accurately and quickly given the latter. The regression maps a set of predictors, derived from the state profiles, onto corresponding values of $\overline{k}$. The predictors are functions of absorber amount, pressure, temperature and viewing geometry.

The regression coefficients linking the predictors and $\overline{k}$ are pre-computed in the following way. Spectrally integrated transmittances $\mathcal{T}_i^{A,D}(p_l, \theta)$ are first computed by MOPABS for an ensemble of training atmospheres representative of a wide range of atmospheric states. The ensemble includes highly polluted planetary boundary layer measurements with high CO and CH_4 mixing ratios[9], as well as model calculations by the MOZART[6] chemical transport model for all seasons and a variety of latitudes. These transmittances determine corresponding values of $\overline{k}$, which are tabulated. The predictors for each training atmosphere are also tabulated.

The regression coefficients are computed through a least-squares fit over the ensemble after first mapping $\overline{k}$ and the predictors onto an absorber amount grid, from pressure levels in physical space. Since $\overline{k}$ depends most strongly on absorber amount, which is then already accounted for, the regression is able to focus largely on the weaker dependencies of $\overline{k}$ on pressure and temperature. This method improves the overall accuracy of the fit. The resulting j-th regression coefficient on absorber level m, for gas g, is denoted C_{jm}^g. This completes the pre-calculation of C_{jm}^g.

At run time, the predictors for a given test atmosphere are calculated on each pressure level, then transformed to absorber amount space where the regression coefficients are applied. For the test atmosphere, denote the j-th predictor on absorber level m for gas g by $Z_{jm}^{g,test}$. Then the effective absorption coefficients for the test atmosphere are given by linear equations of the following form:

$$\overline{k}_m^{g,test} = C_{m0}^g + \sum_{j=1}^{J} C_{mj}^g \; Z_{jm}^{g,test}.$$

A transformation back to physical space yields $\overline{k}^{test}$ on pressure levels. Equation (4) then gives $\mathcal{T}_i^{A,D}(p_l, \theta)$. The TOA radiances and MOPITT instrument signals follow from expressions like Equation (3).

MOPFAS yields channel radiances in good accord with MOPABS calculations. Over a representative ensemble of test atmospheres, MOPFAS and MOPABS have mean differences of 0.05 to 0.1 percent, with maximum differences of 0.4 to 0.7 percent, depending on channel and band. In addition, a MOPFAS calculation is about 10^5 times faster than GENLN2 LBL calculations. The MOPFAS predictors are carefully chosen to maximize their effectiveness for yielding accurate MOPITT channel radiances. This limits the algorithm's use in other contexts, so that MOPFAS performance improvements over MOPABS and LBL occur at the price of specialization.

4. SUMMARY AND FUTURE WORK

A hierarchy of radiation codes has been developed for the MOPITT program which together comprise a powerful and accurate suite of tools to perform MOPITT forward modeling calculations. These codes are undergoing incremental refinement to improve their accuracy and performance. Variants of these codes will also provide a starting point for the development of forward modeling tools for HIRDLS.

An alternate version of MOPFAS is currently being developed using the correlated-k approach. Correlated-k provides a means to reformulate spectral integrations in terms of integrations over smooth absorption coefficient probability distributions. The approximate correlation between distributions at different levels permits pre-calculation of the probability distributions for an appropriate atmospheric ensemble. MOPITT instrument filters can be built into this scheme. At run time an interpolation gives the probability distributions for a given test atmosphere, from which the integrated transmittances are constructed. The technique is physically transparent, yielding an algorithm similar to MOPABS. Further development of this method will be reported in a future publication.

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