

An Improved OPTRAN Algorithm

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Abstract

Presented here is an improved algorithm for the fast and accurate transmittance-calculation procedure, optical path transmittance (OPTRAN). This algorithm combines two techniques developed separately at the NOAA NESDIS and NCEP and implemented in OPTRAN version 7 and 8, respectively. The first technique applies a correction factor to account for the differences between the total transmittances averaged over spectral response function (SRF) and the transmittances that are the product of the SRF-averaged transmittances of individual gases. The correction factor is estimated from a given atmospheric state in a similar way as that to predict transmittances for each gas. The motivation for developing the technique is to eliminate the use of the effective transmittances, a technique difficult to apply in situations when transmittances are estimated for four or more gases. The second technique is developed in order to reduce the number of regression coefficients used to predict the transmittances. It is especially useful for hyper-spectral sensors, such as AIRS, for which the number of coefficients is reduced to 183,106 from 4,280,400 in the previous versions. The technique applies a polynomial function with the gas amount as a dependent variable to estimate the vertical variations of the coefficients, rather than having a separate set of regression coefficients for each vertical layer. We will also present results in improving the computational efficiency for OPTRAN version 8.

1. Introduction

Over the past two decades, the National Environmental Satellite, Data, and Information Service (NESDIS) and National Centers for Environmental Prediction (NCEP) of the Oceanic and Atmospheric Administration (NOAA) have jointly developed an accurate and fast radiative transfer (RT) model (McMillin et al., 1995; Kleespies et al., 2003). The model is an essential component in the NCEP satellite data assimilation system. Its core is a regression-based fast radiative transmittance model, called Optical Path TRANsmittance (OPTRAN). One of its unique features is that the radiative transmittances of an absorbing gas are computed at fixed levels of integrated amount of the gas along the optical path, rather than at fixed pressure levels. OPTRAN has so far eight versions. OPTRAN-V6 (Kleespies et al., 2003) is the current version used in the Global Data Assimilation System (GDAS) at NCEP. Recently, two new versions, OPTRAN-V7 (Xiong et al., 2003) and OPTRAN-V8, have been developed simultaneously at NESDIS and NCEP, respectively. The latter is currently being evaluated, improved and implemented in GDAS.

Both OPTRAN-V7 and -V8 are developed from OPTRAN-V6, which applies the effective-transmittance technique to account for the instrumental band averaging effect and a fixed multi-layer structure to estimate transmittances at fixed layers. OPTRAN-V7 has replaced the effective-transmittance technique with the correction-factor technique. This change makes OPTRAN more efficient and easier to be extended to include more variable gases. However, it requires the same 300-layer structure as that used in OPTRAN-V6, which needs 300 regression equations and 1800 regression coefficients to estimate transmittances per gas and channel. The large number of regression coefficients, however, is a problem for the current NCEP analysis system to assimilate data from hyper-sensors such as AIRS, due to the limitation of the computer memory capacity. OPTRAN-V8 was initiated to solve the problem. It introduces a polynomial function to fit the absorption coefficients along optical paths and thus does not require the multi-layer structure. As a result, the number of regression coefficients is reduced by a factor of 23. However, OPTRAN-V8 still uses the same effective transmittance technique as that used in OPTRAN-V6, and consequently is difficult to be extended to include more variable gases.

In this paper we report the work to integrate OPTRAN-V7 and -V8 by implementing the correction-factor technique into OPTRAN-V8. We also present results from the work to improve OPTRAN-V8 efficiency. We start with a brief description of OPTRAN-V7 and -V8, and then present the methods and preliminary results, followed by a summary.

2. Description of OPTRAN-V7 and -V8

2.1 OPTRAN-V7

In OPTRAN-V7, the atmosphere is divided vertically into 300 layers along the optical path in the so-called absorber space. The absorber space is a set of discrete integrated gas amount $\{A_i, i=0, 300\}$ with A_0 being the minimum value at the top of the atmosphere and A_{300} the maximum value at the surface. Since three gas types are included in OPTRAN-V7, three absorber spaces are required. The distribution of the levels in the absorber space has large impact on the accuracy of the transmittance estimation (Xiong et al., 2003). Once determined, the absorber space is fixed and applied for any cases. OPTRAN estimates gas transmittances, but they are not predicted directly. The absorption coefficients is predicted directly using the following 5-predictor regression equation,

$$k_i = c_{i,0} + \sum_{j=1}^5 c_{i,j} X_{i,j} \quad (1),$$

where k_i is the absorption coefficient at layer i , and $\{c_{i,j}\}$ and $\{X_{i,j}\}$ are regression coefficients and the predictors, respectively. Then, k_i is converted to layer transmittance τ_i using

$$\tau_i = \exp(-k_i(A_i - A_{i-1})) \quad (2).$$

Note that τ_i is the transmittance averaged over the frequency band with the instrument spectral response function (SRF). The regression coefficient set $\{c_{i,j}\}$ in (1) is obtained from a statistical atmospheric profile ensemble, in which both the dependent variable k_i or τ_i and independent variable $X_{i,j}$ are calculated from the ensemble, with τ_i computed using a line-by-line model and the SRFs. The predictor set $\{X_{i,j}, j=1,5\}$ is selected from a pool of 18 pre-defined predictors. The total transmittance

$\tau_{tot,i}$ is a product of three gas transmittances, multiplied by a correction factor τ_c as (for simplicity the layer index i is dropped),

$$\tau_{tot} = \tau_{dry} \tau_{H_2O} \tau_{O_3} \tau_c \quad (3),$$

where τ_{H_2O} and τ_{O_3} are the water vapor and ozone transmittances, respectively, and τ_{dry} is the so-called dry gas transmittance, which includes the contributions from other absorbing gases such CO_2 and CH_4 . The function of τ_c is to correct the difference between the SRF-averaged total transmittance and the product of individual SRF-averaged gas transmittances. Examples of the correction factors are shown in Fig. 1.

The correction factor τ_c is estimated in the same way as that for the gas transmittances, by using (1) and (2). The process also requires an absorber space. It is found that the water vapor absorber space is a good choice for τ_c , although more complicated procedures may be adopted (Xiong et al., 2003).

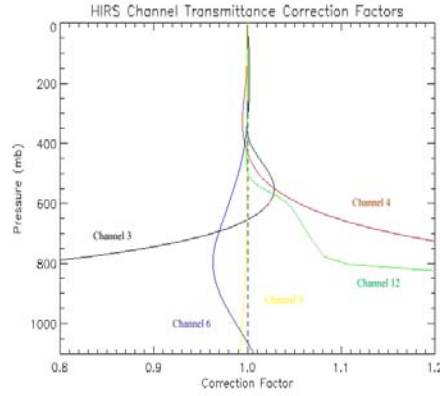


Fig. 1 Correction factors for selected HIRS channels computed using LBLRTM (Clough et al. 1992)

2.2 OPTRAN-V8

In OPTRAN-V8, the multi-layer structure is no longer used. Instead, a single regression equation is applied to predict transmittance at any level as

$$\ln(k(A)) = c_0(A) + \sum_{j=1}^6 c_j(A) X_j(A), \quad (4)$$

where A is the absorber amount of the gas whose transmittances are estimated and $c_j(A)$ is given by a polynomial function as

$$c_j(A) = \sum_{m=0}^{10} a_{j,m} A^m, \quad j = 0, 6$$

where $\{a_{j,m}\}$ is a set of constants. OPTRAN-V8 uses 6 predictors selected from a pool of 17 pre-defined predictors and a 10th order polynomial function. There are total 77 regression coefficients in (4), which is a much smaller number compared with the 2400 coefficients, required by OPTRAN-V7. In practice, instead of using the absorber amount A directly in (4), A is replaced by the following variable,

$$Z = \frac{1}{\alpha} \ln\left(\frac{A-b_2}{b_1}\right), 0 \leq Z \leq 1 \quad (5),$$

where α is a constant determined by trial, and b_1 and b_2 are also constants determined by the minimum and maximum values of the absorber amount A . The absorption coefficient k_c in (4) is related to transmittance by the same formula given by (2), but the transmittance is the effective transmittance, defined in the following,

$$\tau_{tot}^* = \tau_{dry}^* \tau_{H_2O}^* \tau_{O_3}^*, \quad (6),$$

where $\tau_{H_2O}^*$, $\tau_{O_3}^*$ and τ_{dry}^* are the effective transmittances of dry gas, water vapor and ozone, respectively, given by

$$\tau_{dry}^* = \tau_{tot}^* / \tau_{H_2O+O_3}^*,$$

$$\tau_{H_2O}^* = \tau_{H_2O},$$

and

$$\tau_{O_3}^* = \tau_{H_2O+O_3}^* / \tau_{H_2O}^*.$$

The main drawback of the effective-transmittance technique is that it is difficult to be applied for the case in which there are more than three variable gases. In the following section we describe methods to replace the effective-transmittance technique with the correction-factor technique.

3. Implementation of Correction-factor Technique into OPTRAN-V8

The correction-factor technique is first implemented in OPTRAN-V7. As mentioned in the previous section, OPTRAN-V7 treats τ_c as a pseudo transmittance and predicts it in the same way as for the gas transmittances. This treatment simplifies the computing process. With OPTRAN-V8, however, the same treatment does not apply for the following reasons. First, since OPTRAN-V8 predicts $\ln(k)$, not k , it is not valid to treat τ_c as a pseudo transmittance. Secondly, it is found that not all the polynomial modes $\{A^m, m=1,10\}$ in the regression equation have significant contributions for predicting τ_c . The insignificant modes should be dropped to benefit the computational stability. After many experiments, the following regression equation is formulated,

$$\ln(\tau_c) = c_0 + \sum_{j=1}^n c_j X_j \quad (6),$$

where $\{c_i, j=0, n\}$ is a set of constants and $\{X_j, j=1, n\}$ a subset of the 12 predictors listed in Table 1. The accuracy of (6) has been evaluated and the results are shown in Fig. 2 and 3. In these figures, the RMS accuracies are obtained by comparing the OPTRAN-based RT model with a line-by-line model. Fig 2 shows the RMS brightness temperature differences for a subset of AIRS channels computed from both the dependent (blue line) and independent (red line) databases, with the correction-factors estimated using (6) and the gas transmittances calculated exactly. Fig. 3 shows the RMS differences at the HIRS channels from the dependent (Fig. 3a) and independent (Fig. 3b) databases, with both the correction factors and gas transmittances estimated. We see that errors in general are below the 0.1 K level except a few ozone channels.

i	1	2	3	4	5	6	7	8	9	10	11	12
X_i	A_{H_2O}	$A_{H_2O}^2$	$A_{H_2O}^3$	$A_{H_2O}^4$	A_{O_3}	$A_{O_3}^2$	$A_{O_3}^3$	$A_{O_3}^4$	$P^{1/4}$	PT	$A_{H_2O}PT$	$A_{O_3}PT$

Table 1. The set of predictors, from which a subset is selected for estimating the correction factors. A : integrated space-to-layer absorber amount; P : pressure; T : temperature.

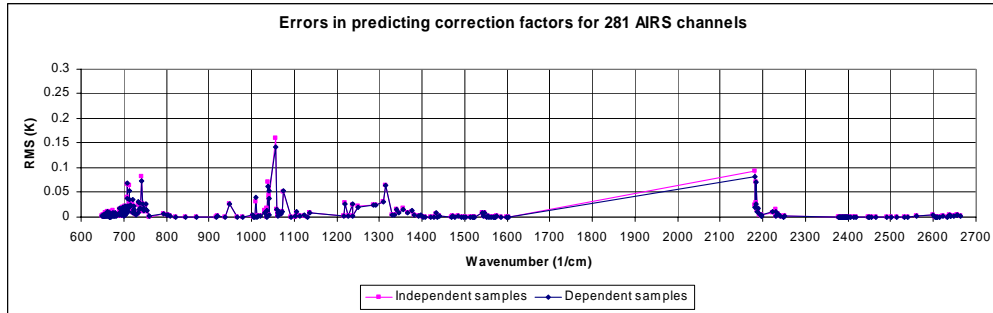


Fig. 2 RMS brightness temperature differences between the OPTRAN-V8 based RT model and the line-by-line mode LBLRTM at the selected 281 AIRS channels. The OPTRAN-V8 model has been modified to include the correction-factor technique. These are the errors from the correction factor only. The gas transmittances are computed exactly using LBLRTM. The independent (red) and dependent (blue) sample sets are based on the CIMSS 32 and UMBC 48 profiles, respectively

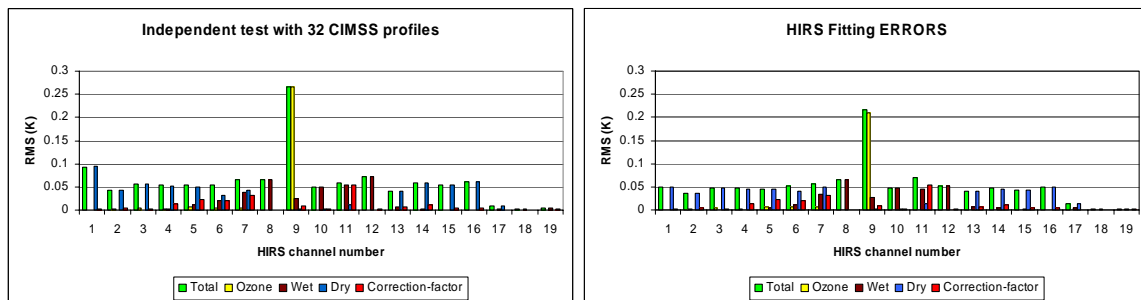


Fig. 3 RMS brightness temperature differences between the OPTRAN-V8 based RT model and the LBLRTM model at the HIRS channels. The OPTRAN-V8 model has been modified to include the correction-factor technique. Fig 3a: the independent data set from the CIMSS 32 profiles; Fig 3b: the dependent data set from the UMBC 48 profiles. Yellow – errors from ozone transmittances; brown – water vapor; blue – dry gas; red – correction factor; green – total transmittances.

4. Efficiency Improvement

Although OPTRAN-V8 uses fewer regression coefficients than OPTRAN-V7, it requires more computational time due to the need to evaluate various polynomial modes. One of the solutions to improve its efficiency is to reduce the order of the polynomial functions under the condition not to decrease the targeted accuracy. Experiment showed that not all transmittance calculations require a 10th order polynomial. For example, for the subset of AIRS channels, only less than 5% of the transmittance calculations need the 10th order polynomial for a targeted fitting error of less than 0.05

K as shown in Fig. 6. Most of the calculations reach this accuracy with a third or second order polynomial function. By varying the order of polynomial functions, we can improve the computational efficiency substantially, as demonstrated in Table 2, which shows a comparison of the time needed to compute the forward RT model and the temperature, water vapor and ozone Jacobians between the fixed 10th order and the varying order polynomial algorithms.

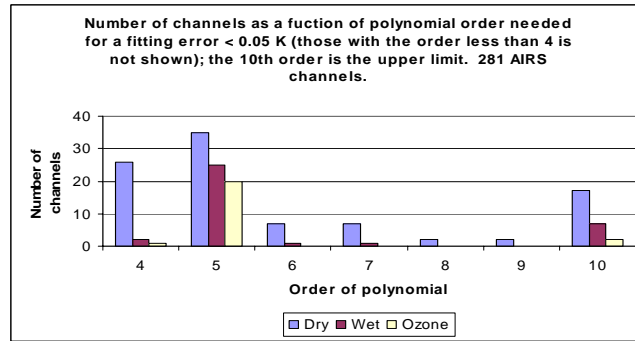


Fig. 4 Number of channels as a function of polynomial order required for estimating radiative transmittances based on a total 281 AIRS channels for a targeted fitting error 0.05 K. Blue - dry gas, red - water vapor, yellow – ozone. The channel distributions for a polynomial order smaller than 4 are not shown in the figure due to their large magnitudes.

	Varied order	Fixed 10th order
Forward model	26 sec	10 min 30 sec
Jacobian	2 min 43 sec	37 min 29 sec

Table 2 Comparisons of time needed for computing forward model and the dry gas, water vapor and ozone Jacobians for 281 AIRS channels between the varying order and fixed 10th order algorithms.

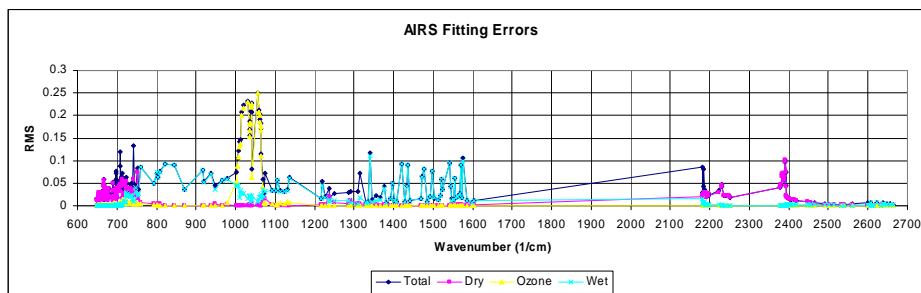


Fig. 5 RMS brightness temperature differences between OPTRAN-V8 based RT model and a line-by-line model at the 281 AIRS channels. The OPTRAN model has been modified to include the varying order algorithm.

5. Summary

We have developed methods to implement the correction-factor technique applied in OPTRAN-V7 into OPTRAN-V8 to account for the difference between the SRF-averaged total transmittances and

the product of the SRF-averaged transmittance components. Our preliminary results show that with these methods the correction factors can be rapidly estimated with an accuracy of better than 0.1 K. We also have done work to improve computational efficiency for OPTRAN-V8. By varying the order of the polynomial function, the computational efficiency can be substantially increased without reducing OPTRAN accuracy.

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