Principal Component-based Radiative Transfer Model (PCRTM)

For Hyperspectral Sensors, Part I: Theoretical Concept

Xu Liu\textsuperscript{a}, William L. Smith\textsuperscript{b} Daniel K. Zhou\textsuperscript{a}, Allen Larar\textsuperscript{a}

\textsuperscript{a}NASA Langley Research Center, MS401A, Hampton, VA 23681, USA

\textsuperscript{b}Hampton University, VA 23668, USA

ABSTRACT

Modern infrared satellite sensors\textsuperscript{1-5} such as AIRS, CrIS, TES, GIFTS and IASI are capable of providing high spatial and spectral resolution infrared spectra. To fully exploit the vast amount of spectral information from these instruments, super fast radiative transfer models are needed. This paper presents a novel radiative transfer model based on principal component analysis. Instead of predicting channel radiance or transmittance spectra directly, the Principal Component-based Radiative Transfer Model (PCRTM) predicts the Principal Component (PC) scores of these quantities. This prediction ability leads to significant savings in computational time. The parameterization of the PCRTM model is derived from properties of PC scores and instrument line shape functions. The PCRTM is very accurate and flexible. Due to its high speed and compressed spectral information format, it has great potential for super fast one-dimensional physical retrievals and for Numerical Weather Prediction (NWP) large volume radiance data assimilation applications. The model has been successfully developed for the NAST-I and AIRS instruments. The PCRTM
model performs monochromatic radiative transfer calculations and is able to include multiple
scattering calculations to account for clouds and aerosols.

Keywords: Radiative transfer model, remote sensing, forward model, hyperspectral data modeling
OCIS codes: 030.5620 and 010.1320

1. INTRODUCTION

With the development of modern remote sensing instruments, progressively higher spectral and
spatial resolution remote sensors are being launched. These modern sensors such as AIRS, TES,
CrIS, IASI, and GIFTS have thousands of channels and provide a wealth of information on
atmospheric and surface properties. The new sensors also present challenges to the analysis of
data. In order to analyze and utilize these vast amounts of data, efficient ways to capture the
information content of the measurements are needed. One of the key components of analyzing
these data is the radiative transfer forward model, which relates the atmospheric states (such as
temperature and trace gas profiles) to the radiances observed from the advanced sensors. Due to
the high spectral resolution, a large number of Radiative Transfer (RT) calculations through the
inhomogeneous atmosphere are needed. Therefore, it will be computationally expensive to
incorporate these data into global NWP data assimilation models using conventional radiative
transfer models. Oftentimes, only subsets of channels are used with existing RT models in order
to handle the corresponding computational constraints.
It is well known that performing line-by-line radiative transfer calculations through the inhomogeneous atmosphere is a very time consuming process. Most molecular gases in the atmosphere have numerous vibrational-rotational transitions, or pure rotational transitions, in the infrared spectral region. Molecular line intensities and shapes are non-linear functions of vertical profiles of atmospheric temperature, pressure and trace gases. Typically one has to divide the inhomogeneous atmosphere into numerous thin layers and use properly weighted atmospheric properties within these layers for the radiative transfer calculations. Since the line widths are very small in the upper atmosphere, the monochromatic calculations are typically done in 0.0001 to 0.0008 wavenumber steps in the infrared spectral region. For example, the TES instrument\textsuperscript{2,5-9} spectral coverage ranges from 650 cm\textsuperscript{-1} to 3050 cm\textsuperscript{-1} with an average frequency grid of 0.0004 cm\textsuperscript{-1}; thus, about 6 million monochromatic radiative transfer calculations are needed to model the whole spectral range.

There are several ways to minimize the computational time needed to perform radiative transfer calculations for the processing of hyperspectral data. One of the approaches, which the TES science team uses, is to store absorption coefficients as a function of atmospheric pressure and temperature at a monochromatic frequency grid in a large lookup table. As a result, the optical depths in a particular atmospheric layer can be calculated simply by interpolations and additions. In this approach, time-consuming calculations of spectral line shapes and intensities are avoided, but the forward model still has to perform numerous monochromatic radiative transfer calculations through inhomogeneous atmospheres in order to obtain Top Of Atmosphere (TOA) radiances. To minimize the calculations needed, the TES science algorithm takes advantage of the high spectral
resolution and high information content of the TES measurements. It selects narrow micro-windows to perform retrievals for a specific trace gas. However, the approach may be sub-optimal in that more channels cannot be used in a simultaneous solution for all desired geophysical parameters.

Another forward model approach is to predict effective layer optical depths by using an efficient fast parameterization. The effective layer optical depth is a channel-averaged quantity, which contains the Instrument Line Shape (ILS) function or Sensor Response Function (SRF); therefore only one radiative transfer calculation per channel is needed. The effective optical depth is derived in such a way that the additive property of optical depth (or the multiplicative properties of transmittances) between different atmospheric layers and different atmospheric gases holds. Equation 1 is an example of how the layer optical depth is calculated:

\[
\tau_{\text{Eff}}^{Ch} (l) = -\ln \frac{\int_{\Delta \nu}^{} \phi(v-v') t_{\text{Mono}}^{Ch}(v,l) dv'}{\int_{\Delta \nu}^{} \phi(v-v') t_{\text{Mono}}^{Ch}(v,l-1) dv'} = -\ln \frac{t_{\text{Ch}}^{Ch}(v,l)}{t_{\text{Ch}}^{Ch}(v,l-1)} = \text{Func} \left[ \sec \theta, T_r, T_z(P,T_r) \ldots \right] \quad (1)
\]

Where \( \tau \) is the effective channel layer optical depth, \( \phi \) is a normalized SRF, \( \Delta \nu \) is the spectral span of the SRF, \( l \) is the atmospheric layer index, \( t_{\text{Mono}}^{Ch} \) and \( t_{\text{Ch}}^{Ch} \) are monochromatic and channel transmittance (space to layer), respectively. \( T_z \) is pressure weighted layer temperature ratio above layer \( l \), and \( T_r \) is the ratio of the layer average temperature to a layer reference temperature. \( \theta \) is the satellite zenith angle and \( P \) is the atmospheric pressure.
There are several fast model parameterizations based on effective optical depth for satellite remote sensing applications\textsuperscript{23,25-30}. Optical Path Transmittance (Optran), Stand-Alone Radiative Transfer Algorithm (SARTA) and RTTOV are three well-known fast models of this kind\textsuperscript{26,27,37}. These approaches have been successfully used in the operational algorithm for HIRS, AMSU, and AIRS data retrievals.

Another method of fast parameterization is to predict channel transmittances or radiances by using a few representative monochromatic transmittances or radiances \textsuperscript{10-16, 19-21, 24, 31,34, 35}. Correlated K Distribution (CKD), Exponential Sum Fitting Transmittance (ESFT), Radiance Sampling Method (RSM) and Optimal Spectral Sampling (OSS) are examples this type of fast RT model approach. Equations 2 and 3 show how the channel radiances or transmittances are calculated.

\[
R_{Ch}(\nu) = \int_{\Delta\nu} \phi(\nu - \nu') R^{Mono}(\nu') d\nu' = \sum_{i=1}^{N} w_i R^{Mono}_{\nu_i} \tag{2}
\]

\[
t_{Ch}(\nu) = \int_{\Delta\nu} \phi(\nu - \nu') t^{Mono}(\nu') d\nu' = \sum_{i=1}^{N} w_i t^{Mono}_{\nu_i} \tag{3}
\]

In the equations, \(R_{Ch}(\nu)\) and \(t_{Ch}(\nu)\) represent channel radiance and transmittance at a center frequency \(\nu\), respectively, and \(w_i\) is the weight for the pre-determined monochromatic radiance or transmittance. Both CKD and ESFT have the advantage of being monochromatic (can extend to include multiple scatterings) and very fast (only a few monochromatic calculations are needed per channel). They are also very accurate for a single atmospheric layer and a single absorption gas.
However, these models are usually trained on one atmospheric layer, and the dependency of channel transmittance on pressure, temperature and gas amounts are introduced later on by assuming a good correlation between vertical layers and no correlation between overlapping gases. Extending them to vertically inhomogeneous atmospheres leads to limited accuracy. Extensive efforts were made in the scientific community to extend these methods to remote sensing applications. One way to overcome this deficiency is to include both layer transmittance and space-to-layer transmittance in the training, and another way is to predict the TOA channel radiance using statistically selected TOA monochromatic radiances (i.e. RMS method). This has the advantage of treating overlapping gases and inhomogeneous layers consistently for all atmospheric layers. The drawback of the RSM is that it needs a relatively large number of monochromatic radiances to approximate TOA channel radiances due to the method used to determine the monochromatic frequency locations. The OSS method developed by AER overcomes this deficiency by fitting TOA channel radiances using a robust ESFT minimization scheme, where typically, one to fifteen monochromatic radiative transfer calculations are needed to predict channel radiance. OSS is also capable of predicting layer or space-to-layer transmittances. Moncet et al have extended the search method to a more robust “Monte Carlo” approach. The OSS fast model is planned to be used to process Cross-track Infrared Sounder (CrIS) and Advanced Technology Microwave Sounder (ATMS) data from future NPP/NPOESS satellites.

All of the fast models described above are channel-based forward models. These models predict channel effective layer optical depths, channel transmittances or channel radiances either by using non-linear functions of atmospheric temperature and gas profiles or through reduced
monochromatic calculations. The PCRTM, on the other hand, does not predict channel radiance directly. Instead, it predicts PC scores, which have much smaller dimension as compared to the number of channels\textsuperscript{14,38,39}. The PCRTM will take advantage of the orthogonal properties of the principal components (PCs) to compress the spectral information (e.g. channel radiance, transmittance or reflectance) into relatively few significant PCs as compared to the number of channels. The observed TOA radiances can be converted to PC scores by projecting the spectrum onto a set of PCs. Conversely, channel radiances can be calculated by linearly combing PCs using PC scores.

2. THEORETICAL BASIS OF PCRTM FORWARD MODEL

For high-resolution infrared spectra, there are a lot of channels that have similar properties. For example, ozone has more than 100000 absorption lines in the spectral range from 600-3000 cm\textsuperscript{-1}. Many of these lines have similar Lorentz or Doppler half-widths. Dependencies of the line intensity and half-width on atmospheric temperature and pressure are similar. All monochromatic radiances are a nonlinear function of atmospheric temperature, moisture and trace gas profiles. The number of independent pieces of information is much less than the number of monochromatic radiances, therefore many radiative transfer calculations are redundant. The PCRTM approach removes this redundancy. The PCRTM will compress channel transmittances or radiances into a set of orthogonal eigenvectors or PCs in a descending order according to the associated eigenvalues. These radiative transfer properties can be easily regenerated via a linear combination of predetermined significant PCs. The linear coefficients are called principal component scores. These PC scores can be obtained by projecting the channel radiances onto each of the PCs. The number of
significant PCs is determined by checking the RMS errors between the original radiances and radiances regenerated using various numbers of PCs. Usually 100-250 PCs are enough to regenerate channel radiances to 0.01 K accuracy for hyperspectral sensors with thousands of channels. These significant PCs capture spectral variations of TOA radiances from one channel to another, while the corresponding PC scores capture the dependencies of spectra on atmospheric temperature and gas profiles. Instead of performing monochromatic calculations at thousands or millions of frequencies in real time, these RT calculations were performed off-line in a training process. Just like other fast forward model trainings\textsuperscript{27,37}, an ensemble of atmospheric profiles, which span the expected range of variability, were selected from a large dataset such as TIGR profile or ECMWF analyses model outputs\textsuperscript{43}. Optical depths at each atmospheric layer were calculated at a monochromatic grid of 0.0001 cm\textsuperscript{-1}. Radiance spectra were generated using layer optical depths under various observation geometries and surface conditions. These monochromatic radiances were then convolved with appropriate sensor response or instrument line shape functions to form channel radiances. A data matrix whose columns consist of N spectra and whose rows consist of channel radiances at M channel frequencies was then formed and a Singular Value Decomposition (SVD) was performed on this matrix. The first PC generated by SVD represents an average channel spectrum. The second PC is orthogonal to the first one and accounts for a major fraction of the variance in the data matrix. Each successive PC is responsible for smaller fraction of the total variance in the data. As mentioned earlier, only a few hundred PCs are needed to regenerate any spectrum in the data matrix. Since these spectra were generated using representative profiles spanning the expected variability of atmospheric and surface conditions, the PCs should be able to represent radiances corresponding to other general atmospheric and surface conditions. Once the PCs are generated, they are pre-stored in the
forward model. The task for the off-line training is to find a good way to predict PC scores, which in combination with PCs produce channel radiances. For a given atmospheric state, PC scores can be predicted using a non-linear function of atmospheric state such as layer average temperature, pressure, water layer amounts etc. As derived below, a better way to predict PC scores is to use a linear function of a few monochromatic transmittances or radiances. It has the advantage that the radiative transfer equation transforms the atmospheric temperature, moisture and trace gas profiles into radiances and these radiances have a linear relationship with the PC scores:

\[ \vec{R}^{ch} = \sum_{i=1}^{N_{pc}} Y_i \vec{U}_i + \vec{e} = \sum_{i=1}^{N_{pc}} \left( \sum_{j=1}^{N_{mono}} a_j R_{j}^{mono} \right) \vec{U}_i + \vec{e} \]  

(4)

In this equation, \( \vec{R}^{ch} \) is the channel spectrum vector, \( \vec{U}_i \) is the \( i^{th} \) PC vector, \( N_{pc} \) is the number of significant PCs. \( Y_i \) is the PC score, which is generated by linearly combining monochromatic radiances \( R^{mono} \) and \( a_j \) are the associated weights. \( \vec{e} \) is a vector containing forward model errors. Usually, the values of \( \vec{e} \) are smaller than 0.04 K. The PC score \( (Y_i) \) is a dot product of PC vectors \( (U_{Nchx1}) \) with the channel radiance vector \( (R_{Nchx1}) \).

\[ Y_i = U_{Nchx1}^{T} R_{Nchx1}^{ch} = \sum_{j=1}^{N_{ch}} u(j,i) \times R^{ch}(j) \]  

(5)

The index \( i \) represents the \( i^{th} \) PC score, \( j \) represents the channel index, the superscript \( T \) stands for transpose, and \( u(j,i) \) is an element of the PC matrix \( (U) \). The channel radiance is a linear combination of monochromatic radiances within the frequency span of that channel. The weights
are simply the normalized ILS or SRF at the monochromatic frequency grid. Both the pre-calculated PC vectors and the ILS (or SRF) do not vary from one atmospheric state to another, therefore, the PC score is a linear function of monochromatic radiances (equation 6).

\[
Y_i = \sum_{j=1}^{nch} U(j,i) \times \left[ \sum_{k=1}^{N} \phi_k R_{\text{mono}}^k (k) \right] = \sum_{l=1}^{N_{\text{max}}} \alpha_l R_{\text{mono}}^l (l) ,
\]

where \( R_{\text{mono}} \) represents monochromatic radiance, \( \phi \) represent normalized ILS (or SRF) and \( \alpha \) is the weight. As mentioned before, there is a lot of redundant information among thousands to millions of monochromatic radiances or transmittances. There is no need to use all of them to predict \( Y_i \) in equation 6. Unlike methods described above, the PCRTM method selects the location of monochromatic frequencies in a very straightforward way by using a correlation function\(^{36} \). Instead of performing a selection within each channel, as is done within OSS, and ESFT models, the PCRTM selection is done in the whole spectral range, thus removing maximum redundant information in the process. The correlation function correctly identifies redundant information; therefore there is no need to perform a labor-intensive search within millions of possible locations. The upper panel in Figure 1 shows an example of correlation coefficients as a function of frequency. The correlation coefficients are converted to vector angles via an arccosine function. The bottom panel is a plot resulting from re-arranging the correlation coefficients according to their magnitudes. The monochromatic radiances were selected by choosing predictors with equal distance in the values of the correlation coefficients. If the correlation coefficients are equal between two monochromatic frequencies, then the corresponding radiance vectors are parallel to each other and contain the same information content. Only one of the points is needed. On the
other hand, if two radiance vectors are orthogonal to each other (i.e. with arccosine of correlation coefficient equals to 90 degree), both should be selected as predictors. The weights \(a_i\) of the selected predictors (monochromatic radiances) are obtained by a simple SVD regression procedure. Usually, only 300-900 terms are needed to predict \(Y_i\) (i.e. for an infrared spectrum ranging from 650 to 3000 cm\(^{-1}\)). The correlation function method in some way is similar to the CKD method in the sense that they both group monochromatic frequencies with similar properties together. In the CKD method, monochromatic frequencies inside the spectral span of an ILS or SRF are re-ordered according to values of molecular absorption coefficients; while in the correlation function method, monochromatic frequencies are re-ordered according to values of correlation functions and it is done over the whole instrument spectral range. The increase in the speed of the PCRTM model comes from two factors: (1) there are less predictants \(Y_i\) to predict due to the PC compression, and (2) there are less overall predictors due to the use of correlation functions in selecting monochromatic frequencies. If the retrieval system uses only PC scores (a few hundreds) not channel radiances (a few thousands), the first factor can lead to an order of magnitude saving in computational time. The second factor is very significant since the PCRTM only performs radiative transfer calculations at a few hundred monochromatic frequencies, while the channel based RTMs perform RT calculations at a few thousand frequencies.

An advantage of the PCRTM model is that no additional effort is required to model spectra with different apodization functions. Since the ILS of a weakly apodized spectrum has ringing and wide ILS spectral span for each channel, the channel based fast RT models\(^{32-34}\) are more difficult to handle as compared to localized ILS. For example, a sinc ILS (or boxcar apodization) will produce negative channel transmittances. One limitation of an OPTRAN type of model is that a
logarithm of a negative effective transmittance (see equation 1) cannot be calculated. For models using monochromic radiances or transmittances as predictors, you have to choose more predictors in order to cover the wide ILS span. This will lead to increased computational time. For PCRTM, the instrument ILS information is captured by the pre-stored PCs. Selection of the predictors is based on the whole instrument spectral coverage to start with, no extra predictors are needed for a weakly apodized spectrum as compared to a strongly apodized spectrum. Another advantage of the PCRTM is that it may be practical to include multiple scattering calculations since a minimum number of monochromatic radiative transfer calculations are needed. The bulk of the multiple scattering calculations are done off-line in the training process. It should be mentioned that for the purpose of retrieval, the PC scores contain all of the essential information on the spectra. The inversion of state vectors can be done in PC domain without having to go to spectral domain. The capability of going to spectral domain is provided mainly for the quality control and for more convenient physical interpretation of the retrieval results.

3. DESCRIPTION OF PCRTM AND PRELIMINARY RESULTS

A flow diagram of the PCRTM model is shown in Figure 2. The model input parameters include eigenvectors for channels spectra, regression coefficients, and absorption coefficients for various atmospheric gases. Since the radiative transfer calculations used to generate predictors for PC scores are done monochromatically, the radiative transfer calculation is very simple and straightforward. In addition to calculating PC scores and channel radiances, the PCRTM is also
capable of providing an analytical Jacobian matrix, which can be used for one-dimensional (1-D) physical retrievals or for 3-D or 4-D variational data assimilations.

The following example shows how the upwelling radiance can be calculated in a clear atmosphere. First, the upwelling radiance (\( R_{v}^{\text{up}} \)) from surface is initiated:

\[
R_{v}^{\text{up}} = \varepsilon_{v}B_{v}(T_{s})
\]  

(7)

In this equation, \( \varepsilon_{v} \) is surface emissivity at frequency \( v \), and \( B_{v} \) is the Planck function at frequency \( v \) and at a given temperature. In this case, the surface thermal emission is calculated at surface skin temperature \( T_{s} \). The upwelling radiance component at sensor altitude and its derivatives with respect to layer temperatures (\( \frac{\partial R_{v}^{\text{up}}}{\partial T_{i}} \)) and trace gas layer amounts (e.g. \( \frac{\partial R_{v}^{\text{up}}}{\partial H_{2}O} \)) can be calculated recursively by starting from the bottom layer:

loop \( l \) from bottom layer to top layer

\[
\frac{\partial R_{v}^{\text{up}}}{\partial \tau_{i}^{0}} = \left[ B_{v}(T_{i}) - R_{v}^{\text{up}} \right] \text{t}_{\text{Top}-1-l} \text{sec(}\theta) \]
\[
\frac{\partial R_{v}^{\text{up}}}{\partial T_{i}} = \frac{\partial R_{v}^{\text{up}}}{\partial \tau_{i}^{0}} \frac{\partial \tau_{i}^{0}}{\partial T_{i}} + (1-t_{i})\text{t}_{\text{Top}-1-l-1} \frac{\partial B_{v}(T_{i})}{\partial T_{i}}
\]
\[
\frac{\partial R_{v}^{\text{up}}}{\partial H_{2}O_{i}} = \frac{\partial R_{v}^{\text{up}}}{\partial \tau_{i}^{0}} \frac{\partial \tau_{i}^{0}}{\partial H_{2}O_{i}}
\]
\[
R_{v}^{\text{up}} = R_{v}^{\text{up}}t_{i} + (1-t_{i})B_{v}(T_{i})
\]

Repeat for next layer
Here, \( l \) represents the layer index, and \( t_l \) and \( t_{n\text{Top}-1-l} \) represent layer transmittance and accumulative top layer to current layer transmittance, respectively; \( \theta \) is the sensor zenith angle. 

\[
\frac{\partial \tau^0}{\partial T} \quad \text{and} \quad \frac{\partial \tau^0}{\partial \text{H}_2\text{O}}
\]

are the derivatives of layer optical depth with respect to layer temperature and layer water column amount, respectively. \( \frac{\partial R_{\text{up}}}{\partial \tau^0_l} \) is the derivative of upwelling radiance with respect to layer optical depth. The superscript \( \theta \) indicates that the transmittance is calculated at a zero zenith angle (i.e. at nadir direction). These two quantities can be easily computed using a lookup table approach\(^5\). Once the monochromatic radiance and associated derivatives are calculated, equation 6 is used to predict the PC scores. If channel radiances are needed, equation 4 can be used to transform information from PC domain to radiance domain.

The PCRTM forward model has been implemented for both AIRS and the NPOESS Airborne Sounder Testbed Interferometer (NAST-I) instruments. The PCRTM fast model has very high accuracy as compared to the line-by-line calculations. Figure 3 shows the RMS and bias errors between the LBLRTM\(^{22}\) and the PCRTM for AIRS instrument for 52 ECMWF diverse profiles at different satellite observation angles. 120 PCs and 246 predictors were used for the AIRS PCRTM model. The RMS errors for the model are usually less than 0.04K.

Figure 4 shows the same model comparison for the NAST-I instrument\(^{40-41}\). There are 8632 channels for the NAST-I instrument; only 200 PCs are needed to represent these channels. To predict the associated 200 PC scores, only 305 monochromatic RT calculations are needed. This means that an average of 0.04 predictors are needed for PCRTM to predict each NAST-I channel.
In contrast, at least one RT calculation and one predictor are needed for each channel for channel-based fast models, requiring a minimum of 8632 RT calculations and predictors. For OPTRAN or SARTA type of fast RTM, each channel needs 10 to 30 predictors to predict the effective channel transmittances. For ESFT, CKD or OSS type fast RTM, 1 to 15 predictors are needed to predict each channel radiance. The PCRTM should have a significant speed advantage as compared to channel-based RTMs.

To test the applicability and accuracy of the PCRTM model, we have compared the observed AIRS radiance with radiance calculated using the PCRTM model. The AIRS spectrum was taken from a clear sky overpass of Aqua over the Atmospheric Radiation Measurement Tropical Western Pacific (ARM-TWP) site on 8 December 2002. The surface pressure and ozone profile are from the European Center for Medium-Range Weather Forecasts (ECMWF) model. Surface temperature is from University of Maryland at Baltimore County (UMBC) retrieval. Water and temperature profiles are mainly from collocated radiosondes over the ARMS-TWP site. The water profile above 200 mb and the temperature profile above 60 mb are taken from the ECMWF model analyses. The surface emissivity spectrum is obtained from the JHU\textsuperscript{42} database. Figure 5 shows the observed AIRS radiance (top panel), the PCRTM calculated radiance (middle panel) and the difference between the two (bottom panel). Large residuals exist near 1050 cm\textsuperscript{-1}. It is clear that the ozone profile from ECMWF analysis does not represent the true atmospheric ozone state. The spikes on the top and bottom panels are due to the undetected “popping” noise of the AIRS instrument detectors. Overall, the agreement is good between the PCRTM calculation and the AIRS observation. It should be mentioned that for this version of the PCRTM, the AIRS SRF is
not the latest available. The channeling and lastest changes in the SRF are now being included in the AIRS PCRTM.

4. DISCUSSION AND CONCLUSIONS

PCRTM is much faster than channel-based RTMs since it predicts PC scores (or “Super Channel” magnitudes) directly instead of channel radiance or transmittance individually. The choice of using radiances or transmittance as predictors is derived theoretically from the properties of PC scores, where the parameterization of PCRTM is physical-based. The accuracy of PCRTM relative to LBL codes is very good, typically less than 0.04K. The accuracy can be improved monotonically to reach that of LBL calculations by increasing the number of predictors. Based on the application of PCRTM to the AIRS and NAST-I instruments, the PC scores can be predicted accurately using a few hundred monochromatic radiances. Channel radiances can be calculated by linearly combining pre-stored PCs with PC scores as weights. The radiance variation as a function of T, H₂O, O₃, CH₄, N₂O, CO, surface emissivity and observation geometry is captured via monochromatic radiative transfer calculations. The redundant spectral information is captured via PC representation. Since RT calculations are done monochromatically, Jacobians can be generated with little extra effort and multiple scattering calculations can be included. The PCRTM provides both PC scores and the associated Jacobian, therefore it is recommended that the physical inversion of state vector be done in the PC domain directly. Information from all channels is transformed into PC scores and the retrieval process can take advantage of maximum information content and retain the best signal-to-noise ratio of the observed spectrum. This way, there is no need to select a sub-set of channels for the sake of computational speed limitation. For quality control,
channel radiances can be generated with a simple PC transformation. Due to its fast speed and high accuracy, PCRTM has great potential for the assimilation of the complete spectrum of observed radiances in NWP. Furthermore, the use of the PCRTM may enable cloud parameters in the NWP operation.

This is one of a series of papers we plan to write for the PCRTM model. The main aim of this paper is to present the theoretical basis of the method and provide some preliminary results. A more detailed description of the model and more results will be presented in future publications.

ACKNOWLEDGEMENTS

This project is supported by funds from NASA and from NPOESS Integrated Program Office (IPO). We would like to thank Atmospheric and Environmental Research (AER) Inc. for providing the Line-By-Line Radiative Transfer Model (LBLRTM) and OSS fast radiative transfer code. We also thank UMBC for providing the NAST-I SARTA model and United Kingdom Meteorology Office for providing ECMWF profiles used in this study.

REFERENCES


Figure 1. Upper panel: Arcccosine of correlation coefficients as a function of frequency, bottom panel: re-arranged according to the magnitudes.

Figure 2. Flow diagram of PCRTM

Figure 3. RMS errors and bias errors of the AIRS PCRTM model relative to LBLRTM

Figure 4. RMS errors and bias errors of the NAST-I PCRTM model relative to LBLRTM

Figure 5. Comparison of the observed AIRS radiance over ARM site on 12/08/2002 with radiance calculated using PCRTM model.
Channel RMS Error using: 200 EOFs and 305 Mono Radiances

Bias Error