Performance assessment of a five-channel estimation-based ice cloud retrieval scheme for use over the global oceans

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This work determines the performance of a five-channel ice cloud retrieval scheme in the context of numerical synthetic experiments and real-world data and examines the implications of these results on the global retrieval of ice cloud microphysical properties over the global oceans. This estimation-based scheme, designed from information content principles, uses a rigorous, state-dependent error analysis to combine measurements from the visible, near-infrared, and infrared spectral regions. In the synthetic experiments, the five-channel scheme performed as well or better in terms of retrieval bias and random error than the traditional split-window and Nakajima and King bispectral retrieval techniques for all states of the atmosphere. Although the five-channel scheme performed favorably compared to the other methods, the inherently large uncertainties associated with ice cloud physics dictate typical retrieval uncertainties in both IWP and effective radius of 30–40%. These relatively large uncertainties suggest caution in the strict interpretation of small temporal or spatial trends found in existing cloud products. In MODIS and CRYSTAL-FACE applications, the five-channel scheme exploited the strengths of each of the bispectral approaches to smoothly transition from a split-window type approach for thin clouds to a Nakajima and King type approach for thick clouds. Uniform application of such a retrieval scheme across different satellite and field measurement campaigns would provide a set of consistent cloud products to the user community, theoretically allowing the direct comparison of cloud properties for the climate processes studies found throughout the literature.


1. Introduction

Cirrus clouds play an important role in the Earth’s climate system through their impact on the Earth’s radiative budget. The precise nature of this radiative effect and its direct consequences on various climate feedback processes, however, are poorly understood due in part to uncertainties in the microphysical properties of the cloud themselves. Satellite missions consequently have devoted a great deal of effort in an attempt to gain a better characterization of the global distribution of these ice cloud properties. A virtual plethora of retrieval schemes based upon both passive and active spaceborne instruments are found throughout the literature [see Miller et al., 2000]. The accuracy of each of these schemes, however, ultimately depends on how well fundamental assumptions used in the inversion technique match real-world conditions [Cooper et al., 2003, 2006; L’Ecuyer et al., 2006]. Deviations of algorithm assumptions from reality are both state and spectrally dependent, meaning both that each retrieval technique will have relative strengths and weaknesses dependent upon the state of the atmosphere and that different retrieval algorithms can yield dramatically different results for a given cloud scene. In this paper, we attempt to address some of these retrieval uncertainty and consistency issues through introduction of a novel multiple-sensor, optimal estimation ice cloud retrieval scheme based upon instrumentation aboard the NASA Afternoon A-Train constellation of satellites.

The work presented here builds upon that of L’Ecuyer et al. [2006] and Cooper et al. [2006], in which a formal information content analysis based upon entropy considerations was used to objectively select the optimal combination of Moderate Resolution Imaging Spectroradiometer (MODIS) measurements for an ice cloud microphysical property retrieval scheme constrained by CloudSat Cloud Profiling Radar (CPR) cloud boundary information. Channel selection was determined through a realistic characterization of not only the sensitivity of top of the atmosphere radiances
to desired retrieval parameters but also to the uncertainties resulting from both the measurements themselves and from the forward model assumptions used in relating observation and retrieval space. The channels selected for the retrieval were strongly dependent upon both cloud and atmospheric properties and the uncertainties characteristic of the observation system. Because of the complexities of these sensitivities to atmospheric state and the need for a fixed retrieval scheme for an operational retrieval, a five-channel retrieval approach was suggested consisting of a combination of error-weighted visible, near-infrared, and infrared channels. Such an approach can be adopted independent of scene since it makes use of the inherent sensitivities in each of these spectral regions to ensure high information content regardless of cloud and atmospheric properties. Tentatively, the 0.64, 2.11, 4.05, 11.0, and 13.3 μm channels were chosen, but it should be noted that any of these channels could be replaced by another channel with similar characteristics with little loss in retrieval information. These results are strictly only valid for the ocean surfaces assumed in the information content studies, however, the general methodology could be applied directly to different surface reflectance functions to determine their impact on the design of an operational retrieval. The optimal estimation based retrieval framework [Rodgers, 1976; Marks and Rodgers, 1993], which allows inclusion of information from multiple sensors and provides a built in set of diagnostics to quantify retrieval and measurement uncertainties, provides the ideal means to implement this flexible, error-weighted retrieval approach.  

[5] Although theoretical information content calculations involving the reduction of entropy between a priori and retrieval states are elucidative, the five-channel retrieval scheme needs assessment in the more practical terms of retrieval performance. Quantification of the performance of this retrieval scheme and investigation of its feasibility at an operational level are the primary focuses of this paper. The optimal estimation retrieval framework as applied to the five-channel approach and quantification of retrieval uncertainties are briefly discussed in section 2. A series of numerical synthetic experiments were performed in section 3 to explore the implications of the uncertainty estimates of section 2 on the performance of five-channel retrieval scheme, essentially quantifying our ability to determine ice cloud properties from current satellite platforms given a realistic assessment of the errors inherent to the ice cloud problem. Synthetic results for the five-channel scheme were also compared to those from other traditional retrieval techniques to examine relative retrieval performance in context of the information content results found in the previous papers. Although these synthetic experiments provide an invaluable tool for testing the behavior of the algorithm under controlled conditions, unfortunately they may be somewhat biased by the fact that similar assumptions are often made in both forward and inverse calculations. These studies must, therefore, be complemented with applications involving real-world observations, as explored in section 4. Because of a lack of a global data set for this algorithm, the retrieval was first applied to MODIS data alone using the MODIS cloud top temperature product as a substitute for CloudSat cloud boundary information. The retrieval algorithm was then applied to a combination of MODIS Airborne Simulator (MAS) and cloud radar and lidar measurements taken during the Cirrus Regional Study of Tropical Anvils and Cirrus Layers—Florida Area Cirrus Experiment (CRYSTAL-FACE). For each data set, the five-channel scheme was compared to more traditional retrieval approaches and operational cloud products when available, where again it is hoped that differences in retrieval results may allow practical insight into both the physics of the ice cloud retrieval problem and into the application of the five-channel retrieval scheme at an operational level.

2. Optimal Estimation Retrieval Framework and Uncertainty Analysis

[5] The optimal estimation retrieval scheme has been discussed frequently [Engelen and Stephens, 1999; Miller et al., 2000; Cooper et al., 2003], but a simple review of the algorithm framework will be included here to facilitate an easier understanding of the merits of the five-channel approach. Letting $\mathbf{x}$ denote the vector of cloud properties to be retrieved, the optimal estimation technique consists of minimizing the quadratic distance between the set of observations, $\mathbf{y}$, and a corresponding set of simulated measurements, $\mathbf{F}(\mathbf{x})$, and that between $\mathbf{x}$ and a suitable a priori guess, $\mathbf{x}_0$, weighted by their respective error covariances. This is accomplished by minimizing the cost function,

$$\Phi(\mathbf{x}, \mathbf{y}, \mathbf{x}_0) = (\mathbf{y} - \mathbf{F}(\mathbf{x}))^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}_0)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_0)$$

with respect to $\mathbf{x}$. $\mathbf{F}(\mathbf{x})$ denotes the physical model relating the cloud parameters to the observations called the “forward model,” $\mathbf{S}_a$ is the a priori error covariance matrix, and $\mathbf{S}_y$ is the measurement error covariance matrix. It is important to note that $\mathbf{S}_y$ represents not only random instrument noise but also the impact of uncertainties in any assumptions used to define the forward model on the simulated radiances $\mathbf{F}(\mathbf{x})$. In the analysis that follows, it will become evident that this often neglected source of uncertainty dominates the performance of the ice cloud microphysical property retrieval in most cases.  

[5] The values of $\mathbf{x}$ for which equation (1) is a minimum can be found by Newtonian iteration assuming a linear or weakly nonlinear problem via

$$\mathbf{x}^{i+1} - \mathbf{x}^i = \mathbf{S}_a \left[ \mathbf{K}_i^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x}^i)) + \mathbf{S}_a^{-1} (\mathbf{x}_0 - \mathbf{x}^i) \right]$$

where

$$\mathbf{S}_a = (\mathbf{S}_y^{-1} + \mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i)^{-1}$$

is the error covariance matrix of the estimated parameters accounting for uncertainties in the forward model, measurements, and a priori data. The Kernel or weighting function matrix, $\mathbf{K}_i$, is the Jacobian of the forward model with respect to the retrieval vector, with elements given by

$$K_{ij} = \frac{\partial F_i}{\partial x_j}$$
The iteration proceeds until such step as the covariance-weighted mean difference between successive estimates is much less than the number of independent variables in the retrieval vector.

[7] In this paper, the optimal estimation approach is applied to three retrieval schemes. In addition to the five-channel scheme of Cooper et al. [2006], both the split-window (SW) scheme [Inoue, 1985; Prabhakara et al., 1988] based upon the infrared 10.8 and 12.0 μm channels and the Nakajima and King (NK) scheme [Nakajima and King, 1990] based upon the visible 0.64 and near-infrared 2.13 μm channels are used extensively. The observation vector for each retrieval includes the radiances for each of the channels used in the retrieval plus an estimate of cloud temperature. The retrieval vector consists of ice water path (IWP), cloud temperature, and effective radius, defined here as

\[ R_e = \frac{3}{4} \frac{\text{Volume}}{\text{Projected Area}} \]  

where the ice clouds were assumed to be composed of randomly oriented randomized hexagonal ice aggregates of Yang and Liou [1998] using the optical properties developed by Baran et al. [2001] and Baran and Francis [2004], arranged in a modified gamma distribution with variance parameter equal to 2. The basis for choosing these crystals is that Baran et al. [2003], on the basis of a method of optimal estimation, showed that the single scattering properties for these aggregates combined with a modified Henyey-Greenstein phase function better explained observed radiances than the optical properties for more pristine crystal habits. With knowledge of IWP and effective radius, it is then straightforward to calculate cloud optical depth for any desired wavelength through knowledge of ice particle size distribution and extinction coefficients. The retrieval of the physical IWP instead of optical depth is of particular interest to those in situ cloud validation and modeling efforts that deal in physical rather than optical space. The retrieval of IWP has an additional benefit in that IWP and effective radius are completely independent, allowing an additional degree of freedom over traditional retrieval schemes that return the highly interdependent values of optical depth and effective radius. Although IWP is not directly dependent upon effective radius, optical depth is through the simple relationship,

\[ \tau = \frac{3}{2} \frac{\text{IWP}}{\rho R_e} \]  

where \( \rho \) is the density of the ice cloud particle.

[8] Both the information content of a set of measurements and the overall performance of the retrieval scheme are dependent upon a rigorous understanding of the forward model and measurement uncertainty, \( \mathbf{S}_r \). The characterization of the forward model and its uncertainties for the five-channel retrieval scheme used for this work has previously been discussed in the formal information content analysis of Cooper et al. [2006]. Instrument error for MODIS primarily results from calibration issues and is on the order of a maximum of a few percent [Guenther et al., 1996]. Error from the forward model assumptions required to simulate radiances, however, is generally much larger. Uncertainties in radiances associated with our choices of ice crystal habit, cloud particle size distribution, and atmospheric temperature and relative humidity profiles were determined by calculating top of the atmosphere radiances for base retrieval assumptions and then comparing these results with radiances found using alternate assumptions. Figure 1 shows the state-dependent nature of these errors for a visible, near-infrared, and infrared channel of the MODIS instrument. Uncertainties in the visible and near-infrared channels are generally much larger than those in the infrared because of the large variability in cloud optical properties associated with different ice crystal habits. Calculation of the state-dependent nature of these uncertainties allows the retrieval scheme to change its \( \mathbf{S}_r \) assumptions as it iterates to its most likely solution for the state vector. Although the base assumption for these studies is that the forward model errors are diagonal matrices, the use of correlations between forward model errors is examined in greater detail in section 3.3. Further uncertainties associated with 3-D radiative transfer effects, multiple-layer clouds, and the vertical inhomogeneity of ice cloud microphysical properties, although certainly important, are beyond the scope of this paper and will be neglected.

[9] Given the large forward model and measurement errors inherent to the ice cloud problem, the precise values selected for the a priori error covariance matrix, \( \mathbf{S}_a \), are important for making an accurate retrieval, yet these quantities are difficult to assign on the basis of our current understanding of the global distribution of ice clouds. Climatologically reasonable values of cloud IWP and effective radius uncertainty are assumed to be 100 g/m² and 25 μm, respectively, unless denoted otherwise. The value for cloud temperature uncertainty is determined by the accuracy of the available cloud boundary information and its selection is discussed separately for each retrieval application used in this paper. Although a priori errors in IWP and effective radius may be correlated, the exact relationship is not entirely obvious from a real-world perspective. The base assumptions for these studies is, therefore, that the \( \mathbf{S}_a \) is diagonal as use of nondiagonal matrices adds information to the retrieval scheme that cannot entirely be justified. The choice of initial guesses for the state vector, \( \mathbf{x}_0 \), are also difficult to assign prior to executing the retrieval. The assumed values of \( \mathbf{x}_0 \) will be discussed separately for each application and potential methods for mitigating uncertainties will be suggested in some cases.

3. Synthetic Studies

[10] A series of synthetic retrievals were performed to quantify retrieval performance for the proposed five-channel optimal estimation based retrieval scheme. Simulated top of the atmosphere radiances were generated for known cloud scenes using an adding and doubling radiative transfer model [Cooper et al., 2006] and then inverted using the optimal estimation retrieval scheme to estimate both retrieval bias and random error. Retrieval bias for the fixed assumptions of these synthetic studies is defined as the difference between the retrieved most likely estimate and truth. The normalized random error is defined as the
square root of the retrieval error variance divided by truth, mathematically,

$$\sigma_i = \frac{(S_{ii})^{1/2}}{x_{\text{truth}}} \times 100$$  \hspace{1cm} (7)$$

where $S_{ii}$ are the diagonal elements of the retrieval error covariance matrix defined in equation (3). Defined in this way, the reported values represent one standard deviation of a probability distribution function of retrieved cloud properties about the most probable estimate.

[11] If the relationship between the top of the atmosphere radiance and the cloud properties is very well defined and does not suffer from nonuniqueness issues, the problem is straightforward and both the bias and random error would be small. For instance, L’Ecuyer et al. [2006] found uncertainties on the order of a few percent for the retrieval of water cloud properties due to the well-constrained physics inherent to that problem. The ice cloud retrieval problem, however, is more problematic in that ice crystal single scatter properties differ dramatically dependent upon the crystal shape, such that retrieval
bias and random error may be largely dependent upon differences between the inversion assumptions and the given state of the atmosphere.

[12] In section 3.1, the magnitude of biases and random errors for the five-channel ice cloud retrieval scheme is quantified given the realistic forward model and measurement error analysis presented in section 2, using the hexagonal aggregates for both the forward and inverse calculations. For this scenario, in which the same optical properties are used in both the forward and inverse directions, any retrieval bias is due to the influence of the a priori information with a magnitude determined by the interaction of forward model sensitivity, a priori guess, and the relative weightings of the forward model and a priori error covariance assumptions. Although one may question the utility of inverting a set of radiances and obtaining an incorrect best estimate, these synthetic retrievals provide a unique state-of-the-atmosphere dependent understanding of the algorithm for real-world retrievals in which truth is not known. Perhaps of even greater importance for these synthetic retrievals are the random error estimates as defined in equation (7), which represent the range of biases that may arise in instantaneous retrievals when inversion assumptions do not match real conditions. This is illustrated by more realistic synthetic retrievals in sections 3.1, 3.2, and 3.3, where the channels adopted, forward model uncertainty, and assumed cloud single scatter properties are altered, respectively, to examine their influence on retrieval performance.

### 3.1. Five-Channel Retrieval Base Results

[13] Synthetic retrievals were run for the five-channel scheme to determine retrieval performance given the realistic forward model and measurement uncertainties inherent to the ice cloud problem. Since these uncertainties impose some level of dependence on a priori assumptions, these experiments were divided into “thin” and “thick” cloud cases to allow a different set of a priori assumptions for each, on the basis of the idea that reflectivities from the CloudSat Cloud Profiling Radar (CPR) used in conjunction with the MODIS measurements would allow for a rudimentary classification of cloud thickness. IWP ranged from 15 to 75 g/m² with an initial guess of 45 g/m² for the thin cloud cases and from 105 to 165 g/m² with an initial guess of 135 g/m² for the thick cloud cases. Effective radius varied from 12 to 36 μm with an initial guess of 24 μm for both thin and thick cloud cases. Although it may be possible to devise a methodology to more accurately constrain a priori cloud properties through either an empirical radar reflectivity-IWP relationship or a passive retrieval scheme, use of a constant a priori has the additional benefit in that it allows an examination of the importance of the initial guess on retrieval performance. The synthetic retrievals were run at each of the 25 combinations of IWP and effective radius listed in Table 1 for each of the thin and thick clouds. For these base cases, the cirrus clouds were placed at 12 km over an ocean surface assuming a McClatchey Tropical atmosphere [McClatchey et al., 1972] with solar zenith and observation angle at nadir. Cloud temperature uncertainty was 1.5 K, consistent with matching CloudSat cloud boundary information to an ECMWF reanalysis temperature profile [Èyre et al., 1993; Cooper et al., 2003].

[14] Figures 2a and 2b show the normalized retrieval bias for IWP and effective radius, respectively, for the thin-cloud experiments using the five-channel retrieval scheme and the forward model uncertainties analysis described in section 2. Retrieval bias is strongly state-dependent but is less than 15% for each IWP and effective radius combination. Figures 2c and 2d show corresponding normalized random error for retrieved IWP and effective radius, respectively. Retrieval random error for both IWP and effective radius are again strongly state-dependent and are generally much larger than the biases with normalized errors ranging from 20 to 50% about the best estimate.

[15] Figure 2 also shows that retrieval biases between IWP and effective radius are clearly correlated, meaning an error in one retrieved parameter induces a corresponding error in the other. This trend is easy to understand in terms of both the estimation-based retrieval scheme and the setup of the forward model. The retrieval scheme attempts to minimize the difference between the observations and the simulated radiances from the forward model as mapped from state space. Modeled radiances are most strongly coupled to optical depth, which is a function of both IWP and effective radius. When the a priori assumptions become important to the final solution and the retrieval begins to deviate from truth, the algorithm allows compensating errors that still allow simulated radiances to somewhat match observations. Figures 3a and 3b show the retrieved and true 0.66 μm optical depth, respectively, for the thin cloud case. Even though the retrieval returned the wrong IWP and effective radius as in Figure 2, these biases compensated to produce an optical depth with errors generally of only a few percent as in Figure 3c. For example, in the 36 μm effective radius cases, retrieved IWP was too small (decreased optical depth) but was compensated by a retrieved effective radius that was also too small (increased optical depth). For cases with large compensating errors that still yield a reasonable optical depth, it is possible to think in terms of the information content analysis of Cooper et al. [2006]. Such cases indicate that only one piece of information, in this case optical depth, can actually be retrieved from the measurements. This concept has potentially important implications for traditional approaches that retrieve both optical depth and effective radius, primarily that although retrieved optical depth may be accurate, estimates of effective radius for these schemes may be highly dubious depending strongly upon the validity of the algorithm cloud microphysical assumptions.

[16] Another way of understanding the relatively small errors in retrieved optical depth is through examination of the off-diagonal elements in the retrieval error covariance matrix, S_e. Since optical depth is a function of both IWP and effective radius, it is necessary to use the correlations.
indicated by $S_y$ to determine total uncertainty in retrieved cloud optical depth in terms of the random error in retrieved IWP and effective radius. In general, the uncertainty in
\[
y = f(x_1, x_2, x_3, \ldots, x_n) \quad (8)
\]
is given by [National Institute of Standards and Technology, 1994]
\[
\delta y = \left[ \sum_{i=1}^{n} \left( \frac{\partial f}{\partial x_i} \right)^2 (\delta x_i)^2 + 2 \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left( \frac{\partial f}{\partial x_i} \right) \left( \frac{\partial f}{\partial x_j} \right) \delta x_i \delta x_j \right]^{1/2} \quad (9)
\]
We find the partial derivative terms through the expression relating optical depth to IWP and effective radius as in equation (5) and the uncertainties, $\delta x_i$, $\delta x_j$, and $\delta x_{ij}$ from the retrieval covariance matrix, $S_x$. Figure 3d shows that the fractional uncertainty in retrieved optical depth is usually under 10% for most of the thin cloud cases. Random errors of up to 25% are found only for the smallest effective radius–large IWP combinations that are furthest from the a priori guess. Thus correlation in errors between IWP and effective radius in the forward model calculations, as
introduced through the $K$ matrix, reduce the optical depth random errors to fractional values generally less than either IWP or effective radius, individually.

[17] Many of the major trends and observations from the thin cloud cases described above are also observed in the thick cloud cases shown in Figure 4. Retrieval bias for the five-channel retrieval approach for the thick cloud cases is again small with discrepancies up to around 15% for both IWP and effective radius. Retrieval random errors for the thick cloud cases are slightly greater than for the thin cloud cases, with errors generally under 30% but up to a maximum of about 50%.
Figure 5. (top) Retrieved and (bottom) normalized random error for IWP for each of the five-channel, SW, and NK schemes.

Figure 6. (top) Retrieved and (bottom) normalized random error for effective radius for each of the five-channel, SW, and NK schemes.
At this point it is reasonable to ask whether or not these results are representative of more traditional channel combinations such as those employed in the SW and NK approaches. While a formal information content analysis based upon entropy principles was used to select the optimal combination of measurements for the five-channel retrieval scheme presented in this work, it is of value to compare the relative performance of this scheme to these other channel combinations within the estimation framework. For simplicity, we consider an effective radius of 26 $\mu$m for IWPs from 15 to 240 g/m$^2$, using constant a priori assumptions of 20 $\mu$m for effective radius and 100 g/m$^2$ for IWP. Figures 5 and 6 compare retrieved IWP and effective radius, respectively, for each of the different retrieval schemes. For both IWP and effective radius, the five-channel scheme performs as well or better in terms of both bias and random error than either of the bispectral approaches. In terms of bias, the five-channel scheme behaves as a combination of the two bispectral approaches, behaving more like the NK approach for thick clouds where infrared sensitivities are small and more like the SW approach for the thinnest cloud case where visible and near-infrared uncertainties are large. Inclusion of the 4.05 $\mu$m channel, however, seems to allow some improvement in terms of bias for the five-channel scheme over both the NK approach for thick clouds and the SW scheme for the thinnest cloud case. Biases in each retrieval technique are generally small for the intermediate cloud cases between an IWP of 30 and 90 g/m$^2$ where each scheme has inherent sensitivity given the a priori guess of 100 g/m$^2$. In terms of random error, however, the five-channel scheme consistently performs better than each of the other retrievals for all states. Normalized random errors are consistently 20 to 30% for the five-channel approach but often exceed 50% when the SW and NK channels are adopted. Thus the biases and random errors presented in Figures 2 and 4 most likely represent a best case scenario and it is reasonable to expect that either the SW or NK techniques will suffer uncertainties that are at a minimum similar if not larger than those predicted by analyzing the five-channel approach.

The presence of biases for these synthetic studies indicates retrieval dependence upon the a priori information and therefore stresses the importance of making the most accurate guess possible for an estimation-based operational retrieval. Furthermore, since retrieval biases for IWP and effective radius are correlated, a good a priori guess in one variable will ultimately improve the retrieval of the other variable. Use of either an empirically derived radar reflectivity-IWP relationship or a bispectral passive approach are obvious possibilities for making a reasonable first guess for the five-channel retrieval scheme, but lie beyond the scope of this work. Although such influence of the a priori on retrieval results may appear to be a negative aspect of the optimal estimation approach, it is important to realize that other retrieval approaches suffer from inversion uncertainties which are rarely considered or reported. Figure 7 shows
that significant retrieval biases also occur for look-up table versions of both the SW and NK approaches when the measurements are contaminated with even a small amount of instrument noise and/or suffer from forward model uncertainties.

The large random errors in Figures 2 and 4 essentially represent the range of “potential biases” for an operational retrieval when inversion assumptions, such as ice crystal habit, do not match real-world conditions. For the ice cloud cases, errors of 50% or more in retrieved cloud properties could be expected for some states of the atmosphere. The relatively large potential biases for both the thin and thick ice cloud cases need consideration in context of operational ice cloud retrieval schemes. Although it is possible that these biases could average out over a large enough sample of measurements, this will only occur if the average set of cloud properties for the sample is known and is implemented in the retrieval scheme. Since a bewildering number of possible ice crystal properties are found throughout the literature, such selection of the appropriate set of cloud properties is unlikely, suggesting a note of caution in the strict interpretation of regional differences in current operational ice cloud products or their temporal trends. A systematic change in ice crystal habit, for example due to changes in upper tropospheric humidity that may impact the environment in which clouds form, may lead to a corresponding error in retrieved cloud properties that will not average out in time. Since this particular example represents the biggest contribution to the potential biases found here, it will be examined in greater detail in the section that follows.

3.2. Effects of Single Scatter Properties

In section 3.1, the hexagonal aggregate ice crystal was used for both the forward and inverse calculations to quantify retrieval performance. Here, to examine the potential biases that may be introduced by errors in the ice crystal habit assumptions, different crystal types were used to generate the synthetic radiances, which were then inverted assuming hexagonal aggregates to estimate cloud properties. These synthetic retrievals attempt to quantify the implications of using the wrong crystal type for a real-world inversion in which the true crystal habit for a given scene cannot be known a priori from the radiance measurement alone.

Figure 8 shows retrieved IWP for each of the (top) five-channel, (middle) NK, and (bottom) SW schemes using different ice crystal habits to generate synthetic radiances for the inversion.
sets of simulated radiances using different ice crystal assumptions. Single scatter properties developed by Yang et al. [2000, 2003] for bullets, columns, rough aggregates, smooth aggregates, and droxtals were employed. A large (small) spread in retrieved cloud properties indicates a strong (weak) dependence upon cloud microphysical assumptions and therefore indicates strong (weak) potential for the retrieval biases to occur at the given state of the atmosphere. For thin clouds with IWP less than about 60 g/m², the five-channel and SW approaches reproduced truth reasonably well in terms of IWP regardless of assumed crystal habit. The NK scheme, however, performs poorly as modeled radiances depended dramatically on the assumed cloud ice crystal habit leading to discrepancies in retrieval results on the order of 100% for the thinnest cloud cases. For thicker clouds, the five-channel and NK approaches perform similarly in the overall spread of retrieved IWP for the different habits, although the five-channel range is consistently centered more about truth. The SW scheme eventually fails for thick clouds as the retrievals converge to the a priori guess, as dictated by the lack of sensitivity for the infrared channels to IWP as the cloud approaches Planck blackbody behavior. Although not shown, results for effective radius agreed in trend with those for IWP.

[24] The retrieval biases for these experiments also provide a qualitative check on retrieval random error presented in Figure 5, which, was argued, represents the ballpark range of expected biases for a given retrieval dependent upon the difference between algorithm assumptions and real-world conditions for a given cloud scene. For the thin cloud retrievals in Figure 5, random errors were largest for the NK retrieval scheme, next largest for the SW scheme, and smallest for the five-channel scheme. These trends agree qualitatively with the spread in retrieved cloud properties as discussed above. It should be noted that uncertainties in ice crystal habit are not the only source of uncertainty, particularly in SW retrievals. Other assumptions such as atmospheric temperature and relative humidity profiles are important for the infrared channels and increase the relative spread in retrieval results shown here when explicitly accounted for. For the thick cloud retrievals in Figure 5, random errors were smallest for the five-channel scheme and approximately similar for the NK and SW schemes. These results agree with the increased spread in retrieved cloud properties about truth for the NK scheme over that of the five-channel scheme. Although the huge SW biases do not seem to match the relatively small random errors found in Figure 5, other diagnostics available to optimal estimation inversion schemes can be used to identify these cases where the SW retrievals clearly failed and collapsed back to the initial a priori assumptions (see, for example, the discussion of the A-matrix by Rodgers [2000]).

3.3. Effects of Error Assumptions

[25] From these results, it is clear that \( \mathbf{S}_e \) will only provide an accurate measure of retrieval error if \( \mathbf{S}_e \) represents a complete accounting of all relevant sources of uncertainty and their variation as a function of the scene being viewed. In fact, the retrieved atmospheric state itself depends on our best estimate of the state-dependent measurement and forward model error as described in section 2. In this section, the magnitude of these errors are altered to examine their influence on overall retrieval performance. The results from the five-channel scheme using the uncertainty analysis of section 2 are compared to those for the five-channel scheme with uniform combined forward model and measurement error of both 5 and 10% independent of wavelength and atmospheric state.

[26] Figure 9 shows retrieval bias and random error in IWP for thin clouds for these three sets of assumptions. The uniform 5 and 10% error cases reduce the uncertainties in the scattering channels and allows the retrieval scheme to take advantage of the large sensitivities found at these wavelengths. As a result, both bias and random error dramatically decrease, except for the very thin optical depth clouds whose forward model uncertainties actually increased by switching to a flat 10% error. Retrieval random errors are generally under 20% for both IWP and effective radius (not shown) except again for the very thin clouds.

[27] Even a casual comparison of these results to those of Figure 8, however, clearly indicates that the 5 and 10% uniform error assumptions are far too optimistic to be representative of forward model uncertainties. In fact, if one were to repeat the ice crystal habit simulations conducted in section 3.2 with either of these error assumptions, one would find that the optimal estimation inversion does not converge to a solution, confirming that these error estimates are unrealistically small. It is, nevertheless, interesting to note that if forward model and measurement uncertainties could be reduced to 5 or even 10% for the visible and near-infrared channels, we could ensure much more accurate retrievals for almost all states of the atmosphere. The obvious difficulty is to determine a way to reduce these uncertainties. Advancements in the determination of real-world cloud properties through a combination of in situ measurements and theoretical modeling along the lines of Yang et al. [2000] and Baran et al. [2001] would reduce the range of expected radiative properties, thus decreasing the magnitude of forward and measurement error covariances. It may also be possible to use multiple observations from several viewing angles to gain some a priori knowledge of the crystal type for a given radiance measurement [Baran et al., 1999; McFarlane et al., 2005], thereby allowing a means to justify reducing the magnitude of the error covariances.

[28] Figure 9 also shows retrieval bias and random error for the best estimate of state-dependent errors when correlations between forward model uncertainties are included in the off-diagonal elements in \( \mathbf{S}_e \). The use of correlations between forward model uncertainties for the MODIS channels can be justified from a physical standpoint in that errors in simulated radiances resulting from error in algorithm assumptions should be similar for related wavelengths. For instance, an incorrect assumption of ice crystal habit that results in too large of simulated radiance at 0.66 \( \mu \)m generally yields a simulated radiance that is too large at 2.13 \( \mu \)m as well. Similarly, incorrect assumptions in the atmospheric temperature profile would result in highly interdependent errors between different infrared channels. Ballpark estimates of error correlations between retrieval channels were estimated using the calculations of the uncertainty analysis of section 2, in which the effects of ice crystal habit, particle size distribution, atmospheric
temperature, and atmospheric relative humidity on calculated simulated radiance were quantified. For the results shown in Figure 9, coefficient correlations of 0.5 and 0.7 were assumed between the visible 0.66 \( \mu m \) channel and the near-infrared 2.13 \( \mu m \) channel and between the 10.8 \( \mu m \) and 13.3 \( \mu m \) channels, respectively. For these synthetic results, the addition of correlations does not have a significant impact on the retrieval scheme, most likely because of the fact that the channels are already linked through the controlled cloud single scattering properties. This is somewhat comforting since it suggests that even though correlated errors are to be expected in the real-world, their inclusion in an operational retrieval suffers from the fact that their true correlation strength is not known.

4. Real-World Studies

[29] Synthetic studies provide an ideal means to examine expected retrieval performance in a controlled manner based upon a given understanding of the physics of the inversion problem. Unfortunately, our best understanding of the physics may not necessarily match real-world conditions. Application of the five-channel algorithm to real-world data is required to investigate the operational feasibility of this retrieval approach, in other words, will the retrieval consistently converge to realistic results given the rigorous error analysis of Cooper et al. [2006]. To this end, in section 4.1, the five-channel retrieval scheme is applied to MODIS data and compared to results from each of the SW and NK techniques as well as to the MODIS operational cloud product [King et al., 1997]. In section 4.2, the five-channel scheme is further tested using a combination of measurements from the CRYSTAL-FACE field campaign and again compared to results from each of the bispectral approaches.

4.1. MODIS Data

[30] The five-channel retrieval scheme presented in this work was based upon an information content analysis for MODIS measurements constrained with coincident CloudSat cloud boundary information. Until data from CloudSat and CALIPSO becomes available, the combination of measurements necessary to evaluate this retrieval scheme at the global scale will not be available. In this subsection, the five-channel retrieval scheme is applied to MODIS radiances alone, using the MODIS cloud top temperature product [Menzel et al., 2002] as a proxy for coincident cloud boundary information. While this retrieval does not exactly reproduce the combined CloudSat-MODIS approach, it does provide an initial satellite-based data set to determine whether the five-channel retrieval scheme can consistently achieve convergence for real-world clouds given cloud microphysical assumptions and the state-dependent nature of the forward model and measurement error matrices. Furthermore, results from the five-channel scheme compared to those from both the bispectral approaches and the MODIS cloud optical depth product should allow a means to determine if the general trends observed in the synthetic studies occur in the real-world.

[31] The five-channel retrieval scheme was applied to MODIS radiances for 5000 ice cloud pixels located over the tropical Indian Ocean, assuming a McClatchey tropical atmosphere. The MODIS cloud top temperature product was used to constrain the infrared radiances, dictating an increase in the a priori uncertainty for cloud emitting temperature from 1.5 K to 5 K. IWP and effective radius
(and thus optical depth) for the five-channel scheme were estimated assuming the forward model and measurement uncertainties of section 2 and constant initial guesses of 20 μm for effective radius and 100 g/m² for IWP. Figure 10 compares inferred optical depth from the five-channel retrieval, optimal estimation implementations of the SW and NK retrieval approaches, and the MODIS cloud optical depth product. Retrieval convergence for the five-channel scheme was generally successful, but to ensure 100% convergence for the scheme it was sometimes necessary to relax the forward model uncertainties for the visible and near infrared channels to 30% when smaller error assumptions resulted in failed convergence. This relaxation indicates that the real-world does not behave quite as cleanly as the assumptions of the synthetic studies suggest, a topic that will be explored in detail in section 4.3. The general trends in retrieved optical depth, however, agree well with expectations from the synthetic results and suggest potential utility in the five-channel retrieval approach at an operational level. The five-channel retrieved optical depth match the SW technique well for thin clouds and match the NK more closely for thick clouds, with an intermediate transition near an optical depth of 4. The MODIS cloud product, which is based upon a non-optimal-estimation NK-type approach but with different cloud microphysical assumptions, retrieves larger optical depths than any of the optimal estimation based approaches for all but the smallest optical depth bin. Although disquieting at first glance, this incongruity in retrieved ice cloud properties is entirely consistent with the analysis of ice crystal habit impacts in section 3.2. It should be noted, however, that we do not imply that either the five-channel scheme or the MODIS optical depth product is more or less correct than the other. The scheme whose assumptions happen to match the real-world best for the given cloud scenes would be more correct. The design of five-channel scheme essentially minimizes the retrieval uncertainty for all states of atmosphere, but as stated in the earlier discussions of retrieval bias and random error, it cannot always guarantee an accurate best guess because of the inherent variability of the physics of the ice cloud retrieval problem.

4.2. CRYSTAL-FACE

[32] The Cirrus Regional Study of Tropical Anvils and Cirrus Layers—Florida Area Cirrus Experiment (CRYSTAL-FACE) of 2002 provides an ideal real-world data set to test the five-channel retrieval scheme. A large number of coincident aircraft, ground-based, and satellite-based observations were taken during CRYSTAL-FACE to meet the ultimate project goal of gaining a better characterization of the role of tropical cirrus clouds in climate processes. For the five-channel retrieval scheme, the relevant measurements to assess the retrieval scheme from CRYSTAL-FACE are the radiances from the MODIS Airborne Simulator (MAS) used in conjunction with either the Cloud Radar System (CRS) or the Cloud Physics Lidar (CPL), all of which were flown aboard the ER-2 research aircraft. Even though a tremendous number of measurements were taken during the campaign, the actual number of test cases available for assessment of our retrieval scheme is limited to relatively few cases which did not grossly violate our error covariance assumptions of single-layer clouds over an
ocean surface. The ER-2 flight leg from 23 July provided just such an ideal validation case. At approximately 1830 UTC, the ER-2 flew over a progressively thickening cirrus cloud shield off the east coast of Florida as indicated by the combined CRS-CPL overlap shown in Figure 11. The increasing 0.66 µm and decreasing 10.8 µm MAS radiances of Figure 12 clearly indicate the presence of an optically variant cloud with a clear jump in visible reflectance corresponding to the lowering of cloud base as indicated by the CRS. This assessment scenario is nearly

![Figure 11](image1.png)

**Figure 11.** Radar (CRS) and lidar (CPL) reflectivities for CRYSTAL-FACE cirrus test case of 23 July. Areas of blue indicate lidar only signal, areas of red indicate radar only signal, and areas of green indicate lidar and radar overlap.

![Figure 12](image2.png)

**Figure 12.** MODIS Airborne Simulator radiances for 0.66 µm and 10.8 µm bands shown for the cirrus test case of Figure 11.
ideal for testing the relative merits of the five-channel retrieval scheme as compared to the two bispectral schemes simply because the range of the observed cloud properties should span the theoretical strengths and weaknesses of each of the bispectral techniques.

Figures 13 and 14 show retrieved IWP and effective radius, respectively, for the five-channel, NK, and SW retrievals from the combined MAS and CRS measurements for the cirrus cloud case shown in Figure 11. The same a priori guess of 20 \( \mu \text{m} \) for effective radius and 100 g/m\(^2\) for IWP was used for each of these retrievals for continuity. Retrieval results are clearly different for each of these approaches, with large differences between the bispectral retrievals for all cloud states. The five-channel retrieval, as in the synthetic studies, tends to agree with the SW approach for thin clouds and with the NK approach for thick clouds. Another interesting feature is the relatively smooth transition of the five-channel results between thin and thick clouds as it essentially shifts from a SW to a NK style approach. This is particularly useful for global applications where a single algorithm that combines the strengths of both the SW and NK approaches is desirable. In terms of optical depth, Figure 15 also suggests that the five-channel retrieval scheme agrees best with the SW for thin clouds and with the NK for thick clouds.

These encouraging real-world results suggest the five-channel retrieval scheme may have utility for real-world data at an operational level. It should again be noted, however, it was necessary to relax the error covariance assumptions to 30% for the scattering channels and 15% for the infrared channels whenever state-dependent error assumptions fell below these levels. In fact, even this relaxation does not always ensure convergence for the NK scheme as indicated by the missing values for four of the thin cloud retrievals as shown in Figures 13–15.

### 4.3. Challenges for Operational Retrievals

Although the results from the MODIS and CRYSTAL-FACE MAS-CRS retrievals seem reasonable in matching expectations from the information content analysis and synthetic studies, it was noted that the both the five-channel and NK retrievals required an initial relaxation of forward model error covariance assumptions to achieve convergence for some of the thin cloud measurements. The implication of these failed retrievals is that the real-world does not entirely match the quantification of potential sources of error as outlined by Cooper et al. [2006]. One likely cause of these discrepancies is the use of a very well defined ocean surface albedo of 10% for the visible channels and 1% for the SWIR and infrared channels in our forward model uncertainty analysis of section 2. Deviations of the real-world albedo from this guess would cause the most difficulties for the thin cloud cases where convergence sometimes failed.

Other possible sources of difficulty in matching observations with expectations are solar and cloud geometry. Neglecting real-world 3-D effects may cause difficulties in matching visible band observations as these channels would be most susceptible to variations in cloud geometry. Another possibility for the observed failures in retrieval convergence for the five-channel scheme is that each of the wavelengths used in the retrieval scheme has its own unique weighting function. Figure 16 shows the weighting functions for a visible, near-infrared, SWIR,
Figure 14. Retrieved effective radius for CRYSTAL-FACE cirrus cloud case using each of the five-channel, NK, and SW approaches.

Figure 15. Retrieved optical depth for CRYSTAL-FACE cirrus cloud case using each of the five-channel, NK, and SW approaches.
and infrared channel for an ice cloud with vertically homogeneous IWP and effective radius. For this cloud, the visible and near-infrared channels essentially see further into the cloud than the SWIR and infrared channel. If effective radius is not constant with height, then each of these channels would be “seeing” a different radius and therefore complicate retrieval convergence, an idea previously explored by Baran et al. [2003]. If so, it should be possible to include a new retrieval parameter which describes the change of effective radius with height such that retrieval convergence is achieved. The use of active information such as radar reflectivity profiles from CloudSat may also help better constrain this problem.

Regardless of specific sources of error, the use of multiple channels in a retrieval necessarily leads to greater chances for the real-world to deviate from the idealized assumptions of the inversion scheme, as represented by the original failure of the five-scheme approach for some of the thin cloud cases.

5. Conclusions

In previous work, a formal information content analysis suggested that the ideal combination of MODIS measurements for an ice cloud property retrieval constrained by CloudSat cloud boundary information was highly dependent upon the state of the atmosphere. Each of the scattering, nonconservative scattering, SWIR, and infrared bands has the potential to be the most useful depending upon exact cloud and atmospheric properties. The use of traditional bispectral schemes that only employ one or two of these spectral regions, such as the NK and SW approaches, therefore cannot always ensure an accurate estimate of cloud properties for global retrievals. A five-channel retrieval scheme was therefore proposed that incorporates measurements from each of these spectral regions to allow an accurate retrieval regardless of state. The use of the flexible optimal estimation based retrieval framework provides the ideal means to properly weight those channels with the most information given the atmospheric state through a rigorous accounting of the forward model and measurement error covariance matrix. In this paper, the implications of retrieval information content are quantified in the more practical terms of retrieval performance for the five-channel scheme and compared to results from more traditional approaches.

The retrieval approaches were applied to both a series of numerical synthetic experiments and real-world MODIS and CRYSTAL-FACE data. The five-channel retrieval approach consistently performed better than either of the bispectral schemes in terms of both bias and random error for retrieved IWP and effective radius in these synthetic studies. It is important to note, however, that even though the five-channel retrieval maximizes information for any given retrieval, the large fundamental uncertainties in the physics of the ice cloud problem result in substantial retrieval errors of near 30 to 40% for both IWP and effective radius. In addition, the fact that these uncertainties are rooted in the representativeness of assumed cloud radiative properties in global retrieval schemes imply that substantial biases may remain in their products even after significant temporal and seasonal averaging. These large uncertainties surely inject a note of caution on a literal interpretation of exact values or small regional or temporal trends found in existing cloud climate products.

When applied to real-world observations, the five-channel retrieval agrees with the NK type approach for thick clouds when emission-based channels have little sensitivity and with the SW approach for thin clouds when the scattering-based channels may produce large biases due to uncertainties in ice crystal habit. Essentially, the five-channel scheme behaves as a combination of the two bispectral approaches, taking advantage of the inherent strengths of

![Figure 16. Weighting functions for each of the visible 0.64, near-infrared 2.13, SWIR 3.90, and infrared 10.8 micron channels for a vertically homogeneous cirrus cloud located over an ocean surface.](image-url)
each scheme through a rigorous determination of the atmosphere-dependent forward model and measurement error covariance matrices. The uniform application of such a five-channel retrieval approach would be beneficial in that it would provide consistency in retrieved cloud products across different satellite and field measurement campaigns, thus allowing the direct comparison of cloud products for the numerous climate processes studies found throughout the literature. Application of this five-channel scheme at the global scale soon should be possible through a combination of measurements from both the MODIS instrument flying aboard Aqua and the CloudSat and CALIPSO satellite missions.

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