Radiative and Microphysical Properties of Cirrus Cloud Inferred from Infrared Measurements Made by the Moderate Resolution Imaging Spectroradiometer (MODIS). Part I: Retrieval Method

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ABSTRACT

An optimal estimation–based algorithm is developed to infer the global-scale distribution of cirrus cloud radiative and microphysical properties from the measurements made by the Aqua Moderate Resolution Imaging Spectroradiometer (MODIS) at three infrared (IR) window bands centered at 8.5, 11, and 12 μm. Cloud-top and underlying surface temperatures, as a priori information, are obtained from the MODIS operational products. A fast-forward model based on semianalytical equations for the brightness temperature is used. The modeling errors in brightness temperature are mainly from the uncertainties in model parameters including surface emissivity, precipitable water, and cloud-base temperature. The total measurement–model errors are well correlated for the three bands, which are considered in the retrieval. The most important factors for the accurate retrieval of cloud optical thickness and the effective particle radius are cloud-top and surface temperatures, whereas model parameter uncertainties constitute a moderately significant error source. The three-band IR method is suitable for retrieving optical thickness and effective radius for cloud optical thicknesses within a range of 0.5–6, where the typical root-mean-square error is less than 20% in optical thickness and less than 40% in effective particle radius. A tropical-region case study demonstrates the advantages of the method—in particular, the ability to be applied to more pixels in optically thin cirrus in comparison with a solar-reflection-based method—and the ability of the optimal estimation framework to produce useful diagnostics of the retrieval quality. Collocated comparisons with spaceborne active remote sensing data exhibit reasonable consistency with respect to retrieved particle size.

1. Introduction

Cirrus clouds cover more than 20% of the earth’s surface and play a major role in the earth’s radiation budget (Liou 1986; Stubenrauch et al. 2006). Various parameterizations of the microphysical processes associated with upper-tropospheric ice clouds in global climate models have led to significant variations in estimating radiative budgets, and improvement in the representation of these clouds within climate models is recognized as a challenge (Waliser et al. 2009). A pressing need exists to better quantify cirrus microphysical properties in global climate modeling. Satellite observations provide unique capabilities to infer the global distribution of cirrus properties and their dependence on meteorological and macrophysical states—in particular, temperature, pressure, and cloud type. The Moderate Resolution Imaging Spectroradiometer (MODIS) operational products for optical thickness and the effective particle radius have been derived by a solar-reflection-based method using visible and near-infrared wavelength bands (Platnick et al. 2003). However, for optically thin cirrus, the aforementioned solar-reflection-based method produces large...
uncertainties in retrieved values due to the assumptions of surface reflection properties and ice crystal habits (shapes) (Cooper et al. 2006; Eichler et al. 2009).

The infrared (IR) split-window method, developed by Inoue (1985), is suitable for thin cirrus, as it is relatively insensitive to uncertainties in surface reflection and particle habits (Cooper et al. 2006). The fundamental principle of the method is that brightness temperatures in the IR window between wavelengths 8 and 13 µm and brightness temperature differences between two different wavelengths primarily depend on cloud optical thickness and the effective particle radius. Several attempts have been made to apply the two-band IR method to local or regional studies (e.g., Parol et al. 1991; Giraud et al. 1997; Katagiri and Nakajima 2004). However, for applications of the infrared method, cloud and underlying surface (land or ocean) temperatures and background atmospheric information are necessary and should be predetermined, which has motivated the development of several variants of the multiband IR method using different data sources with different wavelengths (e.g., Chiriaco et al. 2004). Wang et al. (2011) used three MODIS IR bands at 8.5, 11, and 12 µm to retrieve cirrus optical thickness and effective particle size, measurements made by the Cloud–Aerosol Lidar with Orthogonal Polarization (CALIOP) on board the Cloud–Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) satellite to determine cloud-top height, and the Modern-Era Retrospective Analysis for Research and Applications (MERRA) data for temperature and water vapor profiles, thus, making the application limited to the CALIOP–MODIS collocated pixels.

Optimal estimation (Rodgers 2000) is a powerful inversion method originally used in temperature and humidity sounding, but, in recent years, this approach has been widely used for cloud remote sensing (Cooper et al. 2003; Heidinger and Pavolonis 2009; Watts et al. 2011; Walther and Heidinger 2012; Poulsen et al. 2012). Heidinger and Pavolonis (2009) developed a method using optimal estimation to retrieve cloud-top temperature, effective emissivity, and the spectral emissivity difference parameter (the β parameter), which is primarily a function of the effective particle size, from the Advanced Very High Resolution Radiometer (AVHRR) 11- and 12-µm channels. Information about the cloud-top temperature, as a priori, was obtained from CALIOP. Heidinger et al. (2010) investigated the information content in the infrared channels to estimate cloud-top pressure and showed quantitatively the great ability of the CO2 channels around 13 µm. Poulsen et al. (2012) developed an algorithm for the retrieval of multiple cloud variables from solar to infrared spectra obtained from the Spinning Enhanced Visible and Infrared Imager (SEVIRI), and Watts et al. (2011) demonstrated the possibility of detecting multilayer cloud and separately retrieving the cloud heights and optical thicknesses of upper and lower clouds. Optimal estimation has been recognized as a robust tool for multivariable retrieval from multiple measurement signals, which are common in various modern remote sensing applications.

This study is intended to infer cirrus cloud properties on the global scale and is aimed at demonstrating the methodology of the multiband IR method, error assessment, and some preliminary results including validations. The optical thickness, effective particle radius, and cloud-top and surface temperatures are retrieved from the brightness temperatures in three IR bands at center wavelengths of 8.5, 11, and 12 µm, as well as a priori cloud-top and surface temperatures from the MODIS operational product. Because the present analysis is performed at a resolution of 1 km × 1 km, a significant effort is made to develop an efficient algorithm with the capability to rapidly process data with reasonable, well-quantified uncertainties. The remainder of this paper is organized into four sections. Section 2 presents the forward model and the retrieval method, and section 3 is the error analysis undertaken to evaluate the retrieval performance and characterize the IR method with respect to various error sources. In section 4, a case study for a tropical region is used to demonstrate the strengths of the method. The retrieval results are compared with satellite-based passive and active remote sensing data. Section 5 summarizes the study.

2. The forward model

a. Microphysical model and optical properties of ice particles

Because a forward model for actual satellite data analysis needs to be computationally efficient, an approximate forward model is developed for the study. The single-scattering properties of ice particles are precomputed with data taken from the Yang et al. (2013) data library developed by a combination of the discrete dipole approximation and the improved geometrical optics method for randomly oriented, nonspherical ice crystals. Ice particle habits are prescribed by the Baum et al. (2011) and Cole et al. (2013) general habit mix model (GHM), which assumes size-dependent fractions of nine habits of drxtals, solid and hollow columns, plates, solid and hollow bullet rosettes, column aggregates, and small and large aggregates of plates. The particle surfaces are assumed to be severely rough (Yang et al. 2008), leading to a featureless phase
function typical of cirrus cloud (Baran and Labonnote 2007; Baum et al. 2011). The GHM explains the size-dependent ice water content from in situ observations and polarization measurements from satellites (Baum et al. 2011; Cole et al. 2013). The particle size distribution (PSD) is modeled by a gamma distribution–like function with the parameterization proposed by Iwabuchi et al. (2012).

Band-mean optical properties are tabulated with respect to three IR window bands centered at 8.5, 11, and 12 µm wavelengths (bands 29, 31, and 32). The effective particle radius is defined as \( r_e = 3V/(4A) \) (Foot 1988), where \( V \) and \( A \) are the total volume and projected area integrated over the PSD. Averaging over spectral bands is undertaken by weighting the sensor spectral response function and the Planck function at a temperature of 250 K. The optical properties of ice particles are interpolated from the Yang et al. (2013) data library with respect to the complex index of refraction and the phase parameter (the size parameter multiplied by \( m_r - 1 \), where \( m_r \) is the real index of refraction) because of the temperature dependence of the optical constants of ice in the IR (Iwabuchi and Yang 2011). Figure 1 shows the single-scattering properties of ice particles as a function of the effective particle radius. The extinction efficiency is lowest at band 31 and displays significant temperature dependence at bands 31 and 32. When the effective particle size is small, the single-scattering albedo is high at band 29 compared to the other two bands, and indicates that scattering is relatively important for the 8.5-µm wavelength. The optical properties are represented as a sixth-order polynomial of \( 1/(r_e + 4) \) and tabulated for temperatures of 190, 210, 230, 250, and 270 K. The polynomial coefficients are linearly interpolated from the tabulated values with respect to arbitrary reference temperatures.

b. Brightness temperature model

The present model utilizes semianalytic equations for the computation of IR brightness temperatures, because accurate radiative transfer models (RTMs) are not computationally sufficient for processing global-scale MODIS data. The radiative temperature of the IR window band is composed of three components from clouds, gases, and the surface. Each component is represented in analytic equations, where three assumptions are made: 1) the distribution of ice particles within the cirrus cloud is homogeneous, 2) absorbing gases are present below the cirrus cloud, and 3) the radiative source function in the cloud layer varies linearly with optical thickness from the cloud top. Calculations are performed using the band-mean radiative properties of the atmosphere and surface and band-mean cloud optical properties as

\[
\text{Extinction Efficiency} = \frac{3V}{4A} \quad \text{Effective Particle Radius, } r_e (\mu m)
\]

\[
\text{Single-scattering Albedo} = \frac{1}{r_e + 4} \quad \text{Effective Particle Radius, } r_e (\mu m)
\]

\[
\text{Asymmetry Factor} = \frac{m_r - 1}{r_e + 4} \quad \text{Effective Particle Radius, } r_e (\mu m)
\]
previously described. For each band, the Planck function is computed at the center wavelength and converted to a band-mean Planck function with a second-order polynomial with predetermined coefficients. The coefficients of absorbing gases are empirically determined by fitting to clear-sky radiances calculated by a rigorous radiative transfer model ("RSTAR6B") originally developed by Nakajima and Tanaka (1986, 1988) and routinely refined and maintained at the Atmosphere and Ocean Research Institute of the University of Tokyo. Furthermore, radiances for semitransparent cloud are corrected with an empirical equation, in which the coefficients are predetermined by fitting to the RTM calculations. A detailed description of the forward model is given in the appendix.

The brightness temperature is calculated by inverting the Planck function at the center wavelength (8.54, 11.02, and 12.03 μm for bands 29, 31, and 32, respectively) from the band-mean radiance \( I \), which is represented by a function of several variables:

\[
I = I(\mu, W, e_{sfc}, T_{sfc}, T_{top}, T_{bot}, T_{atm}, T_{opt}, r_e, r_e),
\]

where \( \mu = \cos \theta \) is the cosine of the satellite view angle, \( W \) is the precipitable water, \( T_{sfc} \) is the surface temperature, \( T_{atm} \) is the effective air temperature, \( T_{top} \) is the cloud-top temperature, \( T_{bot} \) is the cloud-base temperature, \( T_{opt} \) is the reference temperature for the optical constants, \( e_{sfc} \) is the surface emissivity, \( T_{IR} \) is the cloud optical thickness at a wavelength of 11.02 μm, and \( r_e \) is the effective particle radius. Water vapor is the major absorbing gas in the three bands, and the effective air temperature is the air temperature averaged over an atmospheric column with weighting by specific humidity. The present forward model offers a closed representation of the smooth variations in radiance with respect to multiple variables (avoiding multidimensional interpolation) and capabilities for straightforward calculation of the derivatives (Jacobian matrix elements) needed in the inversion. A single run of the forward model takes approximately 1 μs on an ordinary desktop computer. Figure 2 shows a typical example of the computed brightness temperature differences (BTDs) between bands 31 and 32 and bands 29 and 31 as functions of brightness temperatures (BTs) at band 31 for various cloud optical thicknesses and effective particle radii. The BTDs at these bands are sensitive to cloud properties when \( T_{IR} = 0.2–6 \). The BTD is basically determined from \( (T_{sfc} - T_{top}) \) and \( r_e \). The BTD sensitivity to \( r_e \) is weaker for larger particle sizes. Different band combinations exhibit different sensitivities to the optical thickness and effective radius, as has been shown in previous studies (Chiriaco et al. 2004; Wang et al. 2011).
For \( r_c = 40 \mu m \), the root-mean-square (RMS) errors are approximately 0.25 K for band 29 and 0.19 K for bands 31 and 32. There is significant correlation between the errors among the three bands.

c. Sensitivity test

The sensitivities of the BTs are tested with respect to various variables. Figure 3 shows the BTDs between bands 31 and 32 for standard and perturbed states. Sensitivity to particle habit is not significant, suggesting that the particle size can be inferred with a high degree of confidence from IR observations. Perturbations in cloud-top and -base temperatures influence the BTs significantly when the cloud is optically thick. A more detailed study of the sensitivity of the 8.5- and 11-\( \mu m \) bands to cloud-top and -base temperatures can be found in Garrett et al. (2009). The BTDs strongly depend on the reference temperature for optical constants, particularly when the effective particle radius is small. Use of optical constants at high temperature (270 K) for cold cirrus (<230 K) results in less variance in the retrieved effective particle radius, with an overestimation for small particles and an underestimation for large particle sizes. Therefore, the appropriate optical constants of ice should be used to determine the effective particle radius. Perturbations in the underlying surface temperature have a significant influence on BTs when cloud is optically thin. A perturbation of 10 mm in the precipitable water had a similar significance to that of a 1-K perturbation in surface temperature. Of all uncertainty factors tested, the BTDs tend to be invariant when the effective particle radius is large, which is important for the accuracy of the retrieved effective particle radius in large-particle cases even with weak sensitivity of the BTD to the effective particle radius.

3. Retrieval method and error analysis

a. Data used

The data used are taken from the MODIS collection 5 products and include the BTs of bands, 29, 31, and 32 in the level 1B product. The features are summarized in Table 1. The measurement noise in the MODIS IR window bands is small, as the noise-equivalent temperature difference (NE\( \Delta T \)) is less than 0.05 K in the MODIS sensor specifications. The noise may be larger than the specification when observing cold targets such as dense high cloud, and bias on the order of 0.1 K may be present at low temperatures (Xiong et al. 2009), whereas the mean bias in bands 31 and 32 is likely less than ~0.1 K (Tobin et al. 2006). Cloud-top temperature and pressure at a resolution of 5 km \( \times \) 5 km is obtained from MODIS level 2 product (MYD06). Cloud-top temperature for high cloud is usually determined by the CO\(_2\) slicing method (Menzel et al. 2008), and the cloud top should be considered to be radiatively effective. Holz et al. (2008) showed that the MODIS data infer cloud pressure at an integrated optical thickness of about 1. For a geometrically thick, transparent cloud such as cirrus, the cloud pressure could be much different than that at cloud top. Accordingly, the RMS error in cloud-top pressure is estimated to be around 50 hPa for single-layer clouds. If high and low clouds layers coexist, the inferred cloud-top pressure is located between the two cloud layers but tends to be weighted toward the upper cloud layer. Holz et al. (2008) showed that the cloud top inferred from the CO\(_2\) slicing could be significantly lower than the upper cloud top in the multilayer cloud cases. The precipitable water and atmospheric profile (air temperature and humidity) are taken from the 8-day-mean level 3 product (MYD08_E3) with 1° spatial resolution (Seemann et al. 2006). Level 3 data are used because level 2 daily data are only available in clear-sky pixels. The 8-day-mean standard deviation for daily observations is used to consider the day–night difference in the atmospheric variables. The 8-day-mean data of the underlying surface are taken from level 3 ocean (L3m_8D_SST_9) and land (MYD11C2) products with 9-km (ocean) and 0.05° (land) resolution. The sea surface temperature is retrieved using the split-window method of Brown and Minnett (1999), for which the RMS error is estimated to be 0.35 K. The sea surface emissivity is calculated from the Fresnel reflectance for a flat ocean surface, assuming the temperature-dependent refractive indices of ocean water (Newman et al. 2005). For satellite zenith angles less than 60°, the effects of wind velocity and multiple scattering at the surface are insignificant on the emissivity at the IR window bands (Masuda, 2012). The land surface temperature and emissivities are retrieved by the physics-based day–night algorithm, which uses seven MODIS bands at wavelengths of 3.7–13.3 \( \mu m \) (Wan and Li 1997). The daily temperature accuracy is estimated to be 1 K in wide ranges of surface and atmospheric conditions, and the emissivity RMS...
FIG. 3. BTDs with respect to BTs for a standard state and various perturbed states. (a) Different ice habit models: solid column (SCOL), column aggregates (CAGG), and the GHM and different (b) $T_{\text{top}}$, (c) $T_{\text{bot}}$, (d) $T_{\text{opt}}$, (e) $T_{\text{sfc}}$, and (f) W values.
error is estimated to be ~0.01 (Wan and Li 1997; Wan et al. 2004; Wang et al. 2008).

When retrieving pixel-by-pixel cirrus properties, missing data are interpolated for pixels at 1-km² resolution from adjacent pixels. The atmospheric and surface products are obtained only for clear-sky pixels, which may introduce biases in the variables if used for the analysis of cloudy pixels. In addition, the coarse spatial resolution and the use of 8-day statistics in several products may reduce the spatial and temporal variability. Therefore, the actual errors at the 1-km scale and the time taken to acquire data may be larger than the error estimates listed in Table 1.

Retrieval by the IR method is used for pixels of potential ice clouds that meet three conditions: 1) cloud-top pressure less than 700 hPa in the operational product generated by the MODIS Science Team (MST), 2) BTDs between bands 31 and 32 larger than 0.2 K, and 3) BTDs generated by the MODIS Science Team (MST), 2) BTDs between bands 29 and 31 larger than 0.5 K.

\( \text{(4)} \)

\[ x = \begin{pmatrix} \ln \tau \\ \ln r_e \\ T_{\text{top}} \\ T_{\text{sfc}} \end{pmatrix}, \quad y = \begin{pmatrix} T_{B29} \\ T_{B31} \\ T_{B32} \end{pmatrix}, \quad \text{and} \quad b = \begin{pmatrix} \mu \\ e_{\text{sfc}} \\ W \\ T_{\text{bot}} \\ T_{\text{opt}} \\ T_{\text{atm}} \end{pmatrix}. \]

The problem to be solved can be formulated as

\[ y = F(x, b) + e, \quad \text{(5)} \]

where \( F \) is the forward model and \( e \) is the measurement-model error (see section 3c). The cost function to be minimized is given by

\[ J(x) = (x - x_0)^T S_y^{-1} (x - x_0) + [y - F(x, b)]^T S_y^{-1} [y - F(x, b)]. \quad \text{(6)} \]

where \( x_0 \) is an a priori vector, \( S_y \) is the error covariance matrix of the a priori, and \( S_y \) is the covariance matrix of the measurement-model error.

The prior information and prescribed ranges of the state-vector elements are summarized in Table 2. The assumed \( S_y \) is a diagonal matrix indicating no correlation between errors of the a priori vector elements. The diagonal elements of the matrix are error variances of the a priori. Assuming that little prior information on cloud optical thickness and effective particle radius is available, we try to underconstrain the first two elements in \( x \); thus, the a priori variances for \( \ln \tau \) and \( \ln r_e \) are very large. Prior information on cloud top-temperature \( T_{\text{top}} \) and surface temperature \( T_{\text{sfc}} \) is taken from the MODIS operational product and has limited, known uncertainties. The RMS error of the a priori surface temperature is assumed to be 4 K, and takes into account the error of the product, day-to-day variability within the 8-day period, spatial variability within the coarse-resolution grid, and the effect of low cloud in multilayer cloud situations. If multilayer clouds are present, the retrieved surface temperature will be lower than the actual surface temperature, and the retrieved surface temperature is considered to be the effective surface temperature. In addition to the constraints imposed by the a priori variances,

\[ \text{TABLE 1. Summary of MODIS operational product data used in the retrieval algorithm.} \]

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Level</th>
<th>Spatial resolution</th>
<th>Temporal sampling</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brightness temperature</td>
<td>1B</td>
<td>1 km</td>
<td>Twice per day</td>
<td>NE( \Delta T = 0.05 ) K</td>
</tr>
<tr>
<td>Cloud-top temperature and pressure</td>
<td>2</td>
<td>5 km</td>
<td>Twice per day</td>
<td>( W: ) RMS = 50 hPa (for single-layer cirrus)</td>
</tr>
<tr>
<td>Atmospheric profile</td>
<td>3</td>
<td>1°</td>
<td>8-day mean</td>
<td>( T: ) RMS = 2–5 K</td>
</tr>
<tr>
<td>Precipitable water and air temperature</td>
<td>5</td>
<td>8-day mean</td>
<td>( W: ) RMS = 3.2 mm</td>
<td></td>
</tr>
<tr>
<td>Sea surface temperature</td>
<td>3</td>
<td>9 km</td>
<td>8-day mean</td>
<td>( T_{\text{sfc}}: ) RMS = 1 K</td>
</tr>
<tr>
<td>Land surface temperature and emissivity</td>
<td>3</td>
<td>0.05°</td>
<td>8-day mean</td>
<td>( e_{\text{sfc}}: ) RMS = 0.01</td>
</tr>
</tbody>
</table>

\[ \text{TABLE 2. Prior information and prescribed ranges of the state vector elements.} \]

<table>
<thead>
<tr>
<th>Variable</th>
<th>A priori</th>
<th>Std dev</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ln \tau )</td>
<td>ln1</td>
<td>2.3 (=ln10)</td>
<td>ln0.1</td>
<td>ln12</td>
</tr>
<tr>
<td>( \ln r_e )</td>
<td>ln15.5</td>
<td>1.64</td>
<td>ln2</td>
<td>ln100</td>
</tr>
<tr>
<td>( T_{\text{top}} ) (K)</td>
<td>( T_{\text{top}} )</td>
<td>4</td>
<td>( T_{\text{top}}^\text{opt}: -16 )</td>
<td>( T_{\text{top}}^\text{opt}: +8 )</td>
</tr>
<tr>
<td>( T_{\text{sfc}} ) (K)</td>
<td>( T_{\text{sfc}} )</td>
<td>3</td>
<td>( T_{\text{sfc}}^\text{opt}: -9 )</td>
<td>( T_{\text{sfc}}^\text{opt}: +1 ) (ocean)</td>
</tr>
<tr>
<td>( T_{\text{sfc}}^\text{opt}: +3 ) (land)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
upper and lower limits are applied to the retrieval solutions to avoid an unphysical solution and are shown in Table 2.

As mentioned earlier, the forward model used in this study considers a single-layer cloud alone. In a two-layer-cloud case, however, there should be a chance to estimate the upper-cloud properties by regarding the low-cloud-top temperature as an "effective" background surface temperature if the low cloud is optically thick and has a cloud-top temperature that is close to that of the underlying surface. To extend the applicability to such two-layer-cloud cases, the surface emissivity is adjusted. When the effective surface temperature deviates widely from the a priori surface temperature, the retrieved effective surface temperature is more likely close to the temperature at the low-cloud top, assuming that the low cloud is nearly a blackbody. Therefore, the surface emissivity is corrected by linking to a deviation of the effective surface temperature from the a priori value:

\[
\varepsilon_{\text{sfc}} = \varepsilon_i' + 1 - f_e',
\]

where \(f_e\) is 0 for \(T_{\text{sfc}} < T'_{\text{sfc}} - 5\), 1 for \(T_{\text{sfc}} > T'_{\text{sfc}}\), and increases linearly from 0 to 1 with increasing \(T_{\text{sfc}}\) for \(T'_{\text{sfc}} - 5 \leq T_{\text{sfc}} \leq T'_{\text{sfc}}\).

In the present algorithm, cloud-base temperature for the high cloud is parameterized in terms of the cloud-top temperature and cloud optical thickness:

\[
T_{\text{bot}} = T_{\text{top}} + \Gamma H \quad \text{and} \quad H = G \sqrt{\tau},
\]

where \(H\) denotes the geometrical thickness (km), \(G = 2\) km according to lidar measurements (Sassen and Comstock 2001; Sassen et al. 2008), and \(\Gamma = 6.5\) K km\(^{-1}\), providing the maximum thickness of 6 km. The reference temperature for the optical constant of ice is assumed to be an average of the cloud-top and -base temperatures.

The retrieval is first performed for 5-km grids using grid-mean BTs. The solution for the grid mean is used, as a first guess, in the retrieval for individual 1-km\(^2\) pixels. The Levenberg–Marquardt method is used (Rodgers 2000) to minimize the cost function. On average, six iterations of the evaluation of the forward model and the Jacobian matrix (data kernel) are sufficient to obtain a converged solution \((J < \sim 3, \text{where the degrees of freedom } = 3)\). If the cost function is not sufficiently minimized, there is no optimal solution for explaining the measurement by the forward model with the available data and the a priori constraints. This may occur if multilayer, inhomogeneous, and/or water-phase clouds are present; therefore, the retrieval cost is a measure of the retrieval quality. A further feature of the optimal estimation is a self-diagnosis of the uncertainties of retrieved variables. The error covariance matrix of the solution is given by

\[
S_y = (S_u^{-1} + K^T S_y^{-1} K)^{-1},
\]

where \(K\) is the Jacobian matrix.

After the retrieval, pixels with \(\tau \leq 0.1\) are removed by filtration because they are considered too optically thin or a clear sky was diagnosed by the IR method. Filtration also removes pixels with \(r_e \geq 100\) \(\mu m\) because they are likely to be associated with water-phase cloud.

**c. The measurement–model error**

The measurement–model error \((S_y)\) in Eq. (6) originated from the measurement error, the forward model approximation error, and the uncertainty in the model parameters. The three error components are included in the present study:

\[
S_y = S_{y,m} + S_{y,p} + S_{y,fwd},
\]

where \(S_{y,m}\) and \(S_{y,p}\) are the covariance matrices of the measurement error and model parameter uncertainty. An assumed state and the errors in the present analysis are summarized in Table 3. Because the measurement bias was not well quantified, the ambiguity in the calibration is on the order of 0.05–0.1 K. The assumed measurement error is 0.1 K for all three bands and is uncorrelated among bands. The model parameter errors are evaluated by adding Gaussian random noise to the model parameters and running the forward model for perturbed sets of model parameters.
Figure 4 shows the total measurement–model errors as functions of optical thickness and effective radius, simulated by assuming the error sources summarized in Table 3, and excluding the a priori error. The total RMS error is in the range of 0.3–1.2 K for \( \tau = 0.1–10 \) and generally increases with decreasing \( \tau \). The uncertainties of precipitable water and surface emissivity result in large errors when the cloud is optically thin. The errors associated with optically thick cloud mainly arise from the uncertainties of \( T_{\text{bot}} \) and \( T_{\text{opt}} \). By comparing each contribution in Eq. (11), the model-parameter uncertainty is found to be the largest contributor to the total error. The band 29 error for small particle sizes was an exception, with the forward model error contributing to generate a 20% larger total error. A significant positive correlation of the error among the bands is identified, with correlation coefficients higher than 0.9 under most conditions. The exceptions are the correlation coefficients of 0.6–0.9 for bands 29 and 31 and bands 29 and 32 with small particle sizes and \( \tau = 1–6 \). The high correlation is associated with the small BTD error and is important for the accurate retrieval of the effective particle radius.

Additional errors may arise from the inconsistency between the measurements and the assumptions made in the forward model, such as the assumption of a plane-parallel, single-layer homogeneous ice-phase cloud. The multilayer and mixed-phase clouds, vertical and horizontal inhomogeneity within the cloud, and three-dimensional radiative transfer may significantly increase the total error. These errors are not well quantified here, although a few studies have addressed the issue (e.g., Zhang et al. 2010; Watts et al. 2011). The inadequate assumptions may introduce biases in the BTs, whereas the optimal estimation framework assumes a Gaussian error without bias. Although the need for further studies remains, the effects on the retrieval due to the model assumptions should be investigated in validation studies. The present algorithm simply neglects this type of error; hence, if the final retrieval cost is large, there is an opportunity to detect inappropriate model assumptions.

The calculated error covariance matrix is tabulated with respect to the cloud optical thickness and the effective particle radius. In the retrieval, the error covariance matrix is recalculated by interpolating from the lookup table, a trial state from each iteration.

d. Retrieval-error analysis

The retrieval error originated from the error of the a priori cloud-top and surface temperatures in addition to the measurement–model error. Assuming the error sources in Table 3, the retrieval error is evaluated by a retrieval simulation: 1) by assuming state and model parameters, the forward-model-simulated measurements \( y \); 2) noise due to the measurement and forward model errors is superimposed on \( y \); 3) from \( y \) and the noise-superimposed a priori \( x_a \) and model parameters \( b \), a solution \( x \) was inverted; and 4) the retrieval error, \( x - x \), is obtained. For each single state, a sample of 3000 simulations is used to estimate the RMS and the bias of the retrieval error. Using this procedure, the contribution of each error source may be evaluated.

Figure 5 shows the total retrieval errors in \( \tau \) and \( r_e \). It is important to quantify the bias because the bias can remain in the statistics for a large number of samples, while positive and negative errors appearing at the pixel scale are canceled by averaging over many pixels. A large bias appeared near the boundaries of the prescribed solution ranges (\( \tau = 0.1–12 \) and \( r_e = 2–100 \mu m \)), because the retrieved results are strictly constrained within a range, and the retrievals are excluded if a too optically small optical thickness or a too large particle size is retrieved. The optical thickness of the optically thin (\( \tau < -0.2 \)) cloud may be positively biased, and that of the optically thick (\( \tau > 10 \)) cloud may be negatively biased. The \( \tau \) bias was within \( \pm 20\% \) (in relative units) when \( \tau = 0.3–9 \) and \( r_e = 3–80 \mu m \). The effective particle radii of optically thin (\( \tau < 0.3 \)) and thick (\( \tau > 6 \)) clouds with small particle size tend to be positively biased. The \( r_e \) bias is within \( \pm 20\% \) when \( \tau = 0.3–7 \) and \( r_e = 3–40 \mu m \). The statistical results of retrieved cloud properties should be interpreted with caution under conditions with large biases. At the pixel scale, larger positive and negative errors are expected to appear in the retrieval results. As shown in Fig. 5c, the RMS error of \( \tau \) is less than 20% for most cases with \( \tau = 0.5–7 \) and \( r_e = 2–100 \mu m \). A cloud with \( \tau = 0.2 \) will exhibit a \( \tau \) RMS error of 30%–50%. For \( \tau = 0.5–6 \) and \( r_e = 2–100 \mu m \), the RMS error of \( r_e \) was less than 40% (Fig. 5d). It is interesting that there is no rapid increase in the retrieval error of \( r_e \) for \( r_e > 30 \mu m \), whereas the BTD sensitivity to \( r_e \) is low. As expected, the RMS errors are large when the bias error is large.

Additional tests reveal that the error in the a priori cloud-top and surface temperatures influences the general performance of the \( \tau \) and \( r_e \) retrievals, particularly for optically thin (\( \tau < 0.3 \)) and thick (\( \tau > 8 \)) clouds, where the retrieval errors of both \( \tau \) and \( r_e \) are large. For optically thin cloud (\( \tau < 0.3 \)), the measurement error and uncertainty in the precipitable water and surface emissivity also impact the retrieval accuracy. Uncertainty in cloud-base temperature increases the effective particle radius error for optically very thick cloud (\( \tau > 6 \)). Therefore, the use of accurate cloud-top and -base temperatures, surface temperature, emissivity, and precipitable water is important to ensure the accuracy of the IR method. Further tests reveal that the use of three
bands enables more accurate retrievals of the effective particle radius than does the two-band (11 and 12 μm) split-window method when not using prior information about the temperature at the cloud top and background surface (Fig. 5f).

4. Evaluation and validation

A MODIS granule acquired on 1 April 2007 is analyzed with the IR method. The area covered is located over the western Pacific Ocean. Figure 6 shows the observed image (Fig. 6a) and several retrieved quantities with uncertainty estimates. The cloud optical thickness and the effective particle radius in the MST product are shown for comparison. Optically thin cirrus, shown in purple in Fig. 6a, covered a wide area around the points denoted by A and B. The pink pixels represent thick high clouds, and the whitish pixels around point C are water-phase clouds. The broad area with dark yellow pixels in the western part of the image is the sun glint over the ocean.
The MST product missed many pixels with optically thin cloud even over ocean, and the retrieved effective particle radius is available only for pixels with $\tau > \sim 1$. The IR method successfully retrieved cloud properties for optically thin clouds with $\tau < 1$. Moreover, for many pixels, the cloud optical thickness retrieved by the IR method is smaller than that obtained by the MST product. The difference is likely due to the presence of multilayer clouds or that the assumed ice particle habits are inconsistent between the two methods. The IR method infers larger effective radii compared with the MST method. One of the advantages of the optimal estimation framework in remote sensing is that it can automatically produce several diagnostics related to retrieval quality. The error in $\ln(\tau)$ was large in pixels with optically thin clouds, which mostly appear at the edges of cloudy pixel clusters. The error in $\ln(r_e)$ is large in pixels with optically thin and thick clouds ($\tau < 0.3$ or $>7$). These
FIG. 6. Cloud property retrieval results for a case over the oceanic region in the western Pacific at 0355–0400 UTC 1 Apr 2007. (a) False-color images composed of MODIS bands 1 (0.65 μm in red shade), 7 (2.13 μm in green), and 31 (11 μm in blue, component increases with decreasing signal); the CloudSat–CALIPSO track is shown by a yellow line. (b) Retrieved cloud-top temperature. (c),(e) Cloud optical thickness at visible wavelengths and (d),(f) effective particle radius from the MST product and the IR retrieval, respectively. Retrieval-quality diagnostics from the IR method: the estimated RMS errors associated with (g) lnτ and (h) lnre; (i) the correlation coefficient between errors associated with lnτ and lnre; and (j) the total retrieval cost.
results are consistent with the expectations of the error analysis presented in section 3. Interestingly, the errors in $\ln{\tau}$ and $\ln{r_e}$ are strongly correlated (Fig. 6i). Optically thin (thick) clouds display a positive (negative) correlation. The different correlations were separated at around $\tau = 1$. The errors associated with $\tau$ and $r_e$ for optically thin cloud are large and strongly correlated. When $\tau$ is overestimated, $r_e$ is also overestimated, and vice versa. Figure 6j shows the cost in Eq. (6) evaluated for the final solution. The retrieval cost is low enough in most pixels but was high in pixels around point C, where model assumptions are likely not valid. A close inspection of the results indicate that very large effective radii are obtained for multilayer clouds, with a cloud top for the low cloud significantly colder than the a priori surface temperature, where the retrieval cost is high. The water-phase clouds around point C exhibit a very small effective radius ($<12 \mu$m) with a high retrieval cost. Thus, the retrieval cost is useful for detecting inadequate model assumptions.

To compare the IR and MST retrievals more quantitatively, we tried to select collocated pixels with ice-phase, single-layer cloud. Figure 7 shows a joint histogram of the IR and MST retrievals for collocated pixels with $T_{\text{top}} < -40^\circ$C, $J < 6$, $\tau_{\text{IR}} < 10$, and a satellite zenith angle $<45^\circ$. The retrieved optical thickness was strongly correlated, with a correlation coefficient of 0.84 and an RMS difference of 3. The MST optical thickness tends to be larger than the IR retrieval. Note that the MST product is derived assuming the MODIS collection 5 habit mix with smooth particle surfaces (Baum et al. 2005), making the asymmetry factor and optical thickness retrieved by the solar reflection method greater (Yang et al. 2008; Zhang et al. 2009). For the effective particle radius, the IR and MST results produce a very weak correlation, with a correlation coefficient of 0.07 and an RMS difference of
The MST effective radius exhibits a narrow probability distribution in the range of 15–40 \( \mu m \), with a mode around 27 \( \mu m \), but the IR effective radius is distributed in the range of 12–80 \( \mu m \), with a mode around 31 \( \mu m \). The ratio of the MST retrieval to the IR retrieval tends to become high with increasing difference between the IR and MST \( \tau \) retrievals (Fig. 7c). The discrepancies between the IR and MST approaches could be explained by differences in the assumed ice particle habits and surface texture and/or in the weighting functions (Zhang et al. 2010).

A combination of cloud radar and lidar can be used to derive the vertical profiles of cloud properties. Okamoto et al. (2010) developed an algorithm using the CALIOP (lidar) and CloudSat radar to retrieve vertical profiles of ice-cloud microphysical properties including the effective particle radius and extinction coefficient at a visible wavelength for overlapping lidar–radar cloudy volumes. The radar–lidar algorithm used to retrieve ice cloud microphysical properties is applied to the cloudy volume elements, which are determined by the cloud mask scheme using the CloudSat and CALIPSO data (Hagihara et al. 2010). The cloud mask scheme was developed on the basis of cloud masks derived from shipborne 95-GHz cloud radar and lidar observations in the western Pacific Ocean near Japan (Okamoto et al. 2007) and in the tropical western Pacific (Okamoto et al. 2008). Here, we used the approach introduced by Yoshida et al. (2010) for cloud-particle-type discrimination. Being different from the operational CALIPSO products (Hu et al. 2009), Yoshida et al.’s (2010) method enables vertically resolved discrimination of cloud water phase and ice particle orientation. The method uses a ratio \( \xi \) of attenuated backscattering coefficients for two vertically consecutive cloud layers, in addition to the depolarization ratio \( \delta \). Based on criteria for \( \xi - \delta \) relationships estimated from statistics for observations and theoretical simulations by the Monte Carlo method, the method enabled discrimination of several cloud particle types: 1) water clouds, 2) supercooled water, 3) randomly oriented ice crystals, and 4) horizontally oriented plates that exhibit the specular reflection. The radar–lidar algorithm requires the depolarization ratio measured by CALIPSO, in addition to the radar reflectivity factor and the backscattering coefficient at 532 nm. Additional lookup tables for horizontally oriented plates are implemented in order to allow for the coexistence of oriented ice plates and the randomly oriented ice in a single volume. A specular reflection mode in the radar–lidar algorithm could drastically improve the retrieval results.

Based on this algorithm, the ice-cloud product is provided by Kyushu University (KU), Japan. Figure 8 shows a collocated comparison of the IR, ST, and KU products for the case shown in Fig. 6. The original vertical and horizontal resolutions of the KU product are 240 m and 1.1 km, respectively. Because the MODIS pixel is geologically located at zero altitude, a parallax is operating on the MODIS pixel between the ground level and cloud level when the sensor is looking obliquely.
The parallax should be corrected when matching the MODIS pixel and the CloudSat–CALIPSO vertical column. We correct the parallax using the cloud-top height, and all data for comparison are degraded into a 3.3-km horizontal resolution by averaging to reduce the ambiguity due to location matching. Note that the KU retrieval was performed for overlapping radar–lidar parts, excluding the very thin, uppermost part of cirrus cloud and the deepest part of the optically thick cloud. The purplish-pink line in Fig. 8a denotes the cloud-top height estimated from the cloud-top temperature determined by the IR method and the atmospheric profile (temperatures and geopotentials at prescribed pressure levels) in the Japanese 25-yr Reanalysis (JRA-25), a long-term global atmospheric reanalysis (Onogi et al. 2007). As shown in the figure, the cloud top is close to the top level of the overlapping radar–lidar part, normally with a difference of less than 1 km. The particle
size clearly increases from cloud top to base. As in Fig. 8, the ST $r_e$ is significantly smaller than the IR $r_e$ and KU $r_e$ for cirrus clouds at latitudes of 6°–12°.

Figure 9 shows scatterplots of the IR and KU retrievals of particle size for six selected MODIS granules acquired on 1 April 2007. The KU values are (a) column average with weighting by the extinction coefficient and (b) the values at the cloud top. The vertical error bars denote the 1-$\sigma$ uncertainties diagnosed by the IR method.

5. Summary and conclusions

An optimal estimation-based algorithm is developed for the retrieval of cirrus radiative and microphysical properties using three MODIS IR window bands centered at wavelengths 8.5, 11, and 12 $\mu$m. Information about cloud-top and underlying surface temperatures, as a priori, is obtained from the MODIS operational products. The single-scattering properties of ice particles are calculated using a state-of-the-art scattering data library and the latest knowledge about ice particle size and habit distributions. The forward model is based on semianalytical equations, which are used to compute the IR brightness temperatures and are computationally efficient for global-scale applications. The BT modeling error due to the approximations is small, but larger errors exist due to the uncertainty of the model parameters, including surface emissivity, precipitable water, cloud-base temperature, and the reference temperature for the optical constants of ice. We suggest that the appropriate optical constants of ice should be used to determine the effective particle radius. The total RMS error in BT is within 1.2 K for $\tau$ = 0.1–10 and generally increases with decreasing $\tau$. A significant positive correlation of the error among the bands is identified and associated with the small BTD error. The correlation is taken into account in the retrieval method, in which obtaining an optimal retrieval, particularly of effective particle radii, is important. The retrieval errors are also evaluated assuming the error of the a priori cloud-top and surface temperatures in addition to the measurement–model error. The bias and RMS errors are quantified. As the bias can remain in the statistics for a large number of samples, the statistical results of retrieved cloud properties should be interpreted with caution under conditions with large biases. At the pixel scale, larger positive and negative errors are expected to appear in the retrieval results. The most important factors for accurate retrievals are cloud-top and surface temperatures, and model parameter uncertainties are a moderately significant error source. The three-band IR method is most suitable to retrieving the optical thickness and the effective particle radius of cloud with an optical thickness in the range of 0.5–6, where the typical
RMS error at pixel level is less than 20% in optical thickness and less than 40% in effective particle radius.

A case study for a tropical region demonstrates several features of the method. The IR method could be applied to more pixels of optically thin cirrus compared with the retrieval by the solar reflection method (used in the MST product). A collocated comparison shows that the retrieved optical thicknesses from the IR and MST methods are strongly correlated, but the IR method tends to infer smaller optical thickness and larger effective radii. It is suggested that the difference in the assumptions made about the ice particle habits primarily influences the retrieved quantities. Collocated comparisons with satellite-based active remote sensing show a reasonable correspondence of retrieved particle size. The current IR retrieval of \( r_e \) is close to the radar–lidar retrieval of \( r_e \) at the cloud top. However, this study provides validation results only for limited cases, and more validation work is both necessary and ongoing.

An advantage of the optimal estimation framework is that it can provide a useful set of diagnostics of the retrieval quality. The errors in ln \( r_e \) and ln \( r_e \) are strongly correlated, and optically thin (thick) clouds display a positive (negative) correlation. The correlation of errors will be useful information when comparing the retrieval with that obtained by other methods and when using the retrieval results to evaluate climate models. The retrieval cost is useful for detecting inadequate model assumptions such as multilayer cloud and contamination by water-phase cloud. Compared with the solar reflection method, the multiband IR method has advantages in retrieval accuracy for optically thin cirrus cloud, shows weak sensitivity to ice-particle habits, and is applicable to both daytime and nighttime retrievals. A subsequent report (Part II) will present a global survey of the properties of high-level ice clouds using the multiband IR method.

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### APPENDIX

#### Equations Used in the Forward Model

The upward radiances \( I \) at the top of the atmosphere is decomposed into three components associated with a cloud layer \( (I_{cld}) \), background atmosphere \( (I_{atm}) \), and underlying surface \( (I_{sfc}) \) in the form

\[
I = I_{sfc} + I_{atm} + I_{cld}. \tag{A1}
\]

The radiative transfer in the cloud is simulated with the scaled optical thickness and single-scattering albedo of the cloud by using the similarity principle (Joseph et al. 1976; Liou 2002), as follows:

\[
\hat{\tau} = (1 - \omega g)\tau \quad \text{and} \quad \hat{\omega} = (1 - g)\omega, \tag{A2}
\]

\[
\omega = \frac{1 - \omega g}{1 - \omega g}, \tag{A3}
\]

where \( \tau \), \( \omega \), and \( g \) are the original optical thickness, single-scattering albedo, and asymmetry factor, respectively. The cloud component is calculated by

\[
I_{cld} = E(\hat{\tau}/\mu|J_{\text{top}},J_{\text{bot}}). \tag{A4}
\]

The emerging radiances \( E \) from a cloud layer, in which the radiative source function varies linearly from \( d \) at the downstream boundary to \( u \) at the upstream boundary, is

\[
E(x,d,u) = d - ue^{-x} + (u - d)\frac{1 - e^{-x}}{x}. \tag{A5}
\]

For the thermal emission, the source function at the cloud top–base is

\[
J_{\text{top} - \text{bot}} = (1 - \hat{\omega})B(T_{\text{top} - \text{bot}}), \tag{A6}
\]

where \( B \) is the Planck function. The contribution of scattering to the IR radiance is generally weak and is semiempirically included in the total source function.

The atmospheric component is calculated by

\[
I_{atm} = [D_1 + D_2 B(T_{atm})(1 - e^{-\tau_{atm}/\mu})]e^{-\hat{\tau}/\mu}, \tag{A7}
\]

where \( D_1 \) and \( D_2 \) are coefficients, \( \tau_{atm} \) is the gaseous absorption optical thickness parameterized in a quadratic equation with respect to the precipitable water, and \( T_{atm} \) is an effective mean air temperature

\[
T_{atm} = \frac{T(p)\rho(p)\, dp}{\rho(p)\, dp}, \tag{A8}
\]
where $T(p)$ denotes the air temperature at pressure $p$ and $\rho$ denotes the volume mixing ratio of the water vapor.

The surface component is a sum of thermal emission from the surface and the reflection of downw ard radiance at the surface:

$$I_{sfc} = [B(T_{sfc})e^{sfc}] + I_{sfc,dn}(1 - e^{sfc}) \exp(-\tau_{atm}/|\mu| - \hat{\tau}/|\mu|) \quad \text{and}$$

$$I_{sfc,dn} = D_3 + D_4 B(T_{atm})(1 - e^{-\tau_{sfc}|\mu|}) + E(\hat{\tau}|\mu|_0, J_{bot}, J_{top})e^{-\tau_{sfc}|\mu|_0},$$

where $D_3$ and $D_4$ are coefficients and $\mu_0 = 1/1.66$.

After evaluating the radiance in (A1), an empirical correction is applied:

$$\chi' = a_0 + a_1 \chi + a_2 \chi^2 + a_3 \chi^3,$$

where $a$ is a coefficient and

$$\chi = \frac{T_{sfc} - B^{-1}(I)}{T_{sfc} - T_{top}},$$

The brightness temperature is obtained by

$$T_b = T_{sfc} - (T_{sfc} - T_{top})\chi'.$$

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