Remote sensing of cloud properties using PACE SPEXone and HARP-2: Uncertainties and validation

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# Introduction

Here we discuss the uncertainty estimates and validation approaches for the cloud droplet size distributions (DSDs), cloud phase indices and ice shape and scattering properties derived from the Level-1C data of the PACE polarimeters. Three sources of uncertainty for these products are considered. Firstly, instrument noise and calibration errors may impact the cloud products. Secondly, imperfections of the multi-angle colocation to a single cloud (top) element may lead to retrieval errors. For example, movement of clouds during the timespan of the multi-angle data acquisition may lead to different cloud elements to be observed by different collocated views. Furthermore, the multiple views of the PACE polarimeters are by default collocated with the assumption that the target footprint is on the Earth’s surface, which, in the case of clouds, lead to different cloud elements to be observed by different collocated views depending on cloud height and structure. The third source of uncertainty to be considered is from uncertainties and biases in the assumed physical and optical model of the cloud in the applied radiative transfer model. For example, sub-pixel horizontal and vertical variation of the cloud properties may be ignored in the optical model, potentially causing biases. Furthermore, 3-dimensional radiative transfer effects may be ignored.

We also consider the fact that a product needs to be properly interpreted and information needed for this interpretation may not always be available or is uncertain itself. For example, a retrieved effective radius of the DSD of all clouds in the footprint may not correspond to a simple average of effective radii observed in the same footprint at higher spatial resolution, but rather is a more complex weighted average. Furthermore, the DSD that is retrieved generally represents the value at some (optical) depth within the top of the cloud and knowledge of this probing depth is needed for the proper interpretation of the product.

According to the consideration discussed above, here we discuss the uncertainties of the PACE polarimeter cloud products, the product interpretation and means of (further) validation. We assume all products are retrieved from the hyper-angular HARP-2 observations at 670 nm.

# Drop size distribution using parametric approach

In brief, the cloud top droplet size distribution is inferred from observed polarized reflectances as a function of scattering angle using the equation

Here is the phase matrix element that depends on DSD and is calculated using Mie theory. Generally, the DSD is assumed to be described by a modified gamma distribution defined by an effective radius () and effective variance (). This equation is fitted to the measurements by adjusting coefficients a, b and c using a linear regression. Then, the and combination that leads to the lowest root-mean-squared difference with the measurements is considered to define the retrieved DSD. This method works if contains observations in the ‘cloudbow region’ between 135˚ and at least about 155˚ at an angular resolution of 2˚ or better (Miller et al. 2018).

Note that no radiative transfer calculations are performed for this retrieval. Effects from (3D) multiple scattering on drops, aerosols, air and surface, as well as instrument calibration biases, are assumed to be sufficiently described by Eq. 1. In other words, the relative variations of the cloudbow features from which the size distribution information is extracted are assumed to be not substantially altered by the other effects described above.

The most comprehensive assessment of these assumptions is published by Alexandrov et al. (2012a). They estimated uncertainties in retrieved and caused by multiple scattering, 3D raditive transfer effects, aerosol layers overlying the cloud layer and vertical inhomogeneity of the cloud layer. They concluded is inferred well within 0.5 m by this approach. Furthermore, is inferred within about 30% and is generally biased high because of ignored multiple scattering effects. These conclusions are substantiated by a study with real airborne observations by Fu et al. (2022) and Alexandrov et al. (2016, 2018).

A further assessment of uncertainties by Miller et al. (2018) using 3D radiative transfer simulations generally shows similar uncertainty estimations. Miller et al. (2018) also concluded that uncertainties caused by instrument noise are relatively small and may be neglected. Miller et al. (2018) also demonstrate the robustness of the polarization retrievals against unresolved spatial inhomogeneity, agreeing with previous results from Shang et al. (2015). Note that the conclusions discussed above are based on observations with an angular resolution of about 1˚, while HARP-2 has about 2˚ resolution. However, Miller et al. (2018) showed that 2˚ resolution is sufficient for such retrievals and it can be assumed that the above uncertainties apply.

Alexandrov et al. 2012a and Miller et al. (2018) also assessed the interpretation of the retrieved quantities. One important note is that, in the case of sub-pixel variation of the DSD, the and combination that represent the combined droplet size distribution for the coarse pixel is generally not consistent with the values and that are simply averaged over that pixel (see also Shang et al. (2015). Methods to calculate representative and for a coarse inhomogeneous pixel are described by Alexandrov and Lacis (2000) and Alexandrov et al. (2012a). Furthermore, the retrieved DSD represents the drops at some optical depth from cloud top. Alexandrov et al. (2012a) estimated the retrieved values are generally representative to those at an optical depth of approximately 1. Similarly, Miller et al. (2018) propose a vertical weighting function to interpret the results, which is shown to perform well when applied to simulated observations.

As discussed in the introduction, imperfections of the multi-angle colocation to a single cloud (top) element may lead to retrieval errors. These uncertainties, however, are poorly quantified to date. Biases resulting from colocation of the multi-angle data to the surface instead to cloud top, and from cloud movement during multi-angle data acquisition are subject of ongoing work. Such biases may be substantial in conditions of broken cloud fields with moderately high cloud tops (e.g., congestus), and/or high winds.

The Root-mean-squared difference (RMSD) between the fit and observations, in addition to their Pearson correlation are supplied as potential uncertainty metrics. Retrievals with an unexpectedly high RMSD and/or low correlation are flagged as suspicious or failed retrievals. Such cases may be affected by, e.g., multi-angle colocation errors discussed above.

In situ droplet size distributions for drops with diameters below ~100 micron near cloud top, collocated with a PACE-HARP-2 observation are needed for validation of these products. Furthermore, when direct colocation is not available, validation using statistics, e.g., variation of DSD as a function of cloud top height in a given region, may also be used as validation. Such observations are expected to be available from the PACE-PAX and ARCSIX campaigns, as well as from many other future campaigns. Focus needs to be on the validation of observations in broken and inhomogeneous cloud fields.

# Drop size distribution using Rainbow Fourier Transfer

The Rainbow Fourier Transfer (RFT) method is a technique to infer a droplet size distribution at cloud top from the multi-angle polarimetry without making a priori assumptions on the DSD shape. It is described in detail by Alexandrov et al. (2012b). This method works if scattering angle range contains observations in the ‘cloudbow region’ between 135˚ and at least about 165˚ at an angular resolution of 2˚ or better.

In general, uncertainty sources discussed above in relation to the parametric droplet size distribution retrieval also apply to the RFT method. As performance metric Alexandrov et al. (2012b) use the integrated absolute difference between the true area-normalized DSD and the retrieved size distribution. Generally, the metric is below 10%, while higher errors may occur for narrow distributions with small effective radii (e.g., m and ). Comparisons between DSDs inferred by the Research Scanning Polarimeter (RSP) with in situ observations generally show good agreements for single mode (Alexandrov et al. 2018) and bi-modal (Alexandrov et al. 2020; Reid et al. 2023) DSDs. Importantly, occurrence of bi-modal DSDs in retrievals positively correlates with rain formation (Sinclair et al.).

For validation of this product, similar observations as needed for the parametric DSD retrievals, as discussed above, are needed.

# Cloud phase indices

Detection of the cloudbow in multi-angle polarimetric observations may be considered as a very robust detection of liquid drops at cloud top (rather than non-spherical ice crystals), and hence a robust cloud-top phase determination. Two metrics are derived from the multi-angle polarimetry which parameterize the detection of the cloudbow, namely the liquid index (van Diedenhoven et al. 2012) and a ‘cirrus correlation’, which is the Pearson correlation between the scattering angle and observation at the cloudbow scattering angles. Furthermore, a successful DSD retrieval using the polarimetric cloudbow method (with low RMSD and high correlation) also indicates presence of liquid in the cloud top.

Simulations by van Diedenhoven et al. (2012) show that a liquid layer covered by about 1-2 optical depths of ice is detectable using the liquid index. Unpublished work indicated generally good agreement between cloud top phase determined using a liquid index from RSP and lidar depolarization ratio using the Cloud Physics Lidar. However, further validation and quantification of the uncertainties of these phase indices are needed. Specifically, how the liquid index and cirrus correlation depend on cloud optical depth (for values below about 5), cloud fraction and imperfections of the multi-angle colocation to a cloud top are to be determined. Airborne observations near cloud top using both ice and liquid cloud probes are needed for this. Such observation may be available from the ARCSIX campaign.

# Ice cloud crystal shape and asymmetry parameter

For footprints containing 100% ice-topped clouds, ice crystal shape characteristics and the phase function asymmetry parameter can be inferred from the multi-angle polarized reflectance observations as demonstrated by van Diedenhoven et al. 2012b. Specifically, the mean aspect ratio of hexagonal components of complex ice crystals and mean distortion of the ice away from a smooth hexagonal structure are retrieved (Van Diedenhoven et al. 2012b, 2016). Here, distortion is defined as by Macke et al. (1996) and aspect ratio () is defined as by van Diedenhoven et al. (2016). Observations between about 130˚ and 155˚ scattering angle are needed.

Uncertainties in retrieved asymmetry parameter, aspect ratios and distortion parameters are estimated to be below 5%, 0.1 and 0.1, respectively (van Diedenhoven et al. 2012b, 2016). The retrieved quantities are relatively robust against instrument noise and angular sampling (van Diedenhoven et al. 2012b). The retrievals are affected by Rayleigh scattering and a cloud top height is needed as auxiliary input to correct for this effect. This Rayleigh correction applied to POLDER observations using the 865 nm band had little effect (van Diedenhoven et al. 2020). For PACE-HARP-2, the preferred band may be at 670 nm since it has hyper-angular sampling, but the effect of Rayleigh at this wavelength needs to be assessed. Another source of uncertainty may be the imperfections of the multi-angle colocation to a cloud top, as discussed above.

Application of this method to real observation of RSP and POLDER yielded results that are generally consistent with ice growth theory (van Diedenhoven et al. 2020; van Diedenhoven 2021). Comparisons of the retrievals with in situ observations by van Diedenhoven et al. 2013 showed agreement in some cases, while disagreement in others. Validation of the method is hampered by limited availability of in situ observation of variables that are equivalent to the retrieved products.

Post-launch validation opportunities for ice cloud retrievals may arise from NASA’s ARCSIX campaign, which includes optical ice probes and radiation measurements, and EU’s HALO-South campaign, which includes the PHIPS probe (Abdelmonem et al. 2016). Observations of ice size, shape (component aspect ratios) and/or scattering properties are needed within the top of clouds containing only ice crystals that are reasonably collocated with the PACE-HARP-2 data.

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