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Validation of MUSES NH_3 observations from AIRS and CrIS against aircraft measurements from DISCOVER-AQ and a surface network in the Magic Valley

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S1: MUSES NH_3 a priori profiles

These profiles were derived for TES retrievals from GEOS-Chem global runs (Shephard et al., 2011). They are used for MUSES and CFPR retrievals.

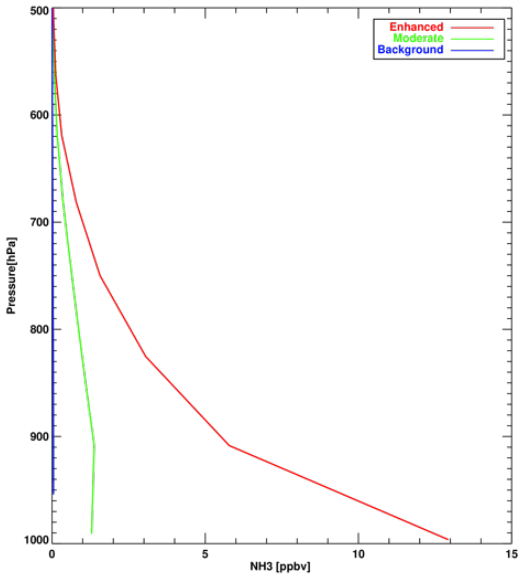

Figure S1: A priori profiles used by the MUSES and CFPR retrievals.

S2: MUSES vs CFPR

The MUSES and CFPR algorithm share many features, as stated in section 2.1, but there are also differences, some of which may be significant (Table S2), such as the inclusion of a cloud optical depth retrieval step and the end-to-end retrieval of the atmospheric state at the pixel level in MUSES. CFPR_v1.6 does provide a cloud flag but does not retrieve cloud optical depth. Both MUSES and CFPR include a preliminary retrieval step to retrieve surface temperature and emissivity. CFPR obtains the atmospheric state (temperature, water vapor) from the NOAA NUCAPS product at the CrIS Field-of-Regard resolution (nine pixels, 42km at nadir), while MUSES retrieves the state from the CrIS radiances at the Field-of-View (FOV or single pixel, 14km at nadir) resolution before running the NH3 retrieval. The MUSES approach ensures that the atmospheric state is derived using the same forward model and radiance data that are used in the NH3 retrieval, reducing, but of course not eliminating, possible sources of error.

Table S1

Product	CFPR (v1.6)	MUSES
Forward Model	OSS	OSS
OE software	IDL ECCC implementation	IDL TROPESS implementation
OE space	Physical	Physical
Levenberg-Marquardt	Yes	Yes
L1 Source	NOAA	NASA
L2 Source	NUCAPS	MUSES
L2 Resolution	FOR	FOV
Cloud retrieval	NO	YES

As a preliminary step in evaluating the differences between the MUSES and CFPR retrievals, each MUSES retrieval used in the DISCOVER-AQ analysis was paired with the corresponding CFPR retrieval (v1.6). The difference plots show that the CPFR product at the surface was biased low with respect to MUSES by ~4 ppbv in California and by ~2 ppbv in Colorado. Determining the source of these differences requires further research.

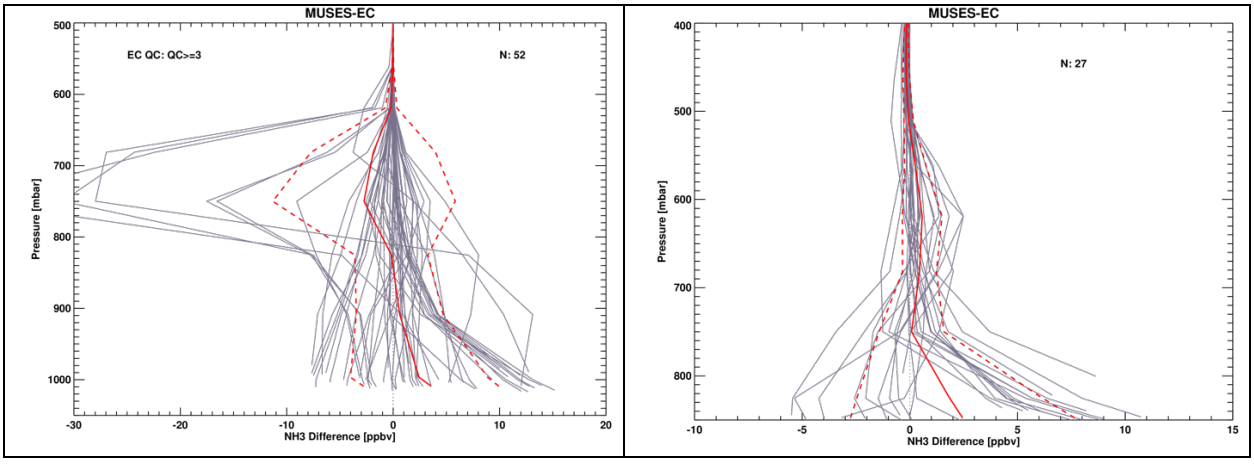

Figure S2: Difference between MUSES and CFPR (EC) DISCOVER-AQ retrieved profiles (grey curves), bias (red curve) and standard deviation (red dashed curves) for California (left) and Colorado(right).

S3: Sample estimated errors from CrIS and uncertainties in aircraft values

Figure S3 shows eight sample profiles retrieved from CrIS radiances during DISCOVER-AQ in California, along with the estimated errors due to the measurement error, (instrument noise), systematic errors and smoothing errors. Note that the errors are added and subtracted to the retrieved profile and plotted cumulatively, in order to highlight the total error: measurement error (light blue), observation error (measurement plus systematic error) (green) and total error (observation plus smoothing error) (orange). The measurement error is by smallest contributor to the total error, while the smoothing error is usually but not always the largest. All profiles except the last were retrieved with the enhanced prior; this case used a moderate prior.

Figure S4 presents the statistics of the aircraft data collocated with each of the retrieved CrIS profiles in Figure S3. The shape of the retrieved profile aligns with the aircraft profile in the first six cases, albeit with the much lower values, consistent with the more limited sensitivity of the retrieval to near surface concentration. In the last two cases the measured profiles did not present the usual drop off across the top of the boundary layer, which the retrieval was not able to capture, even though a reasonable prior was chosen in the last case.

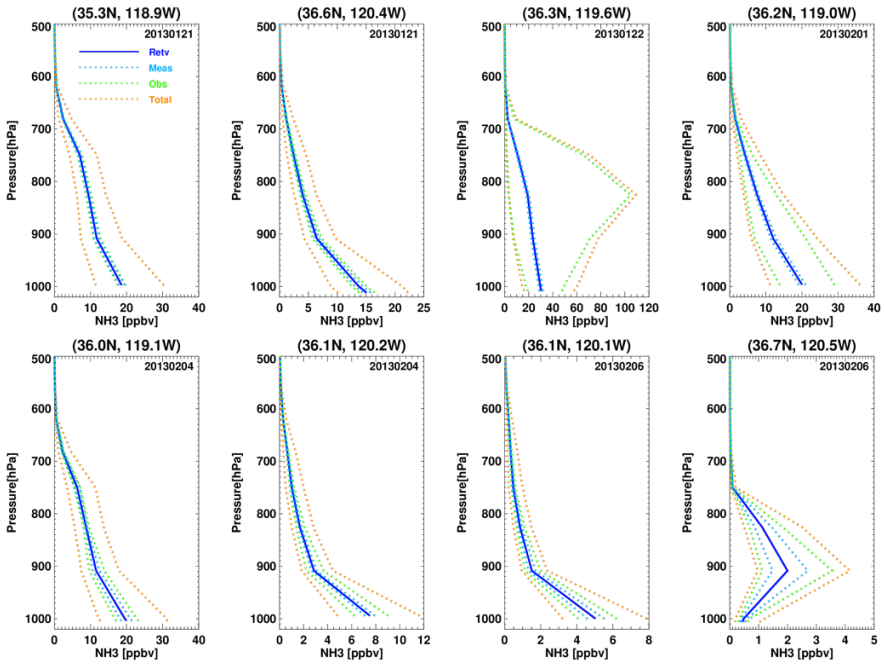

Figure S3: Sample CrIS retrieved profiles from California DAQ and estimated errors: retrieved NH3 (dark blue), measurement error (light blue), observation error (green) and total error (orange). Smoothing error can be inferred from the difference between the total error and the observation error.

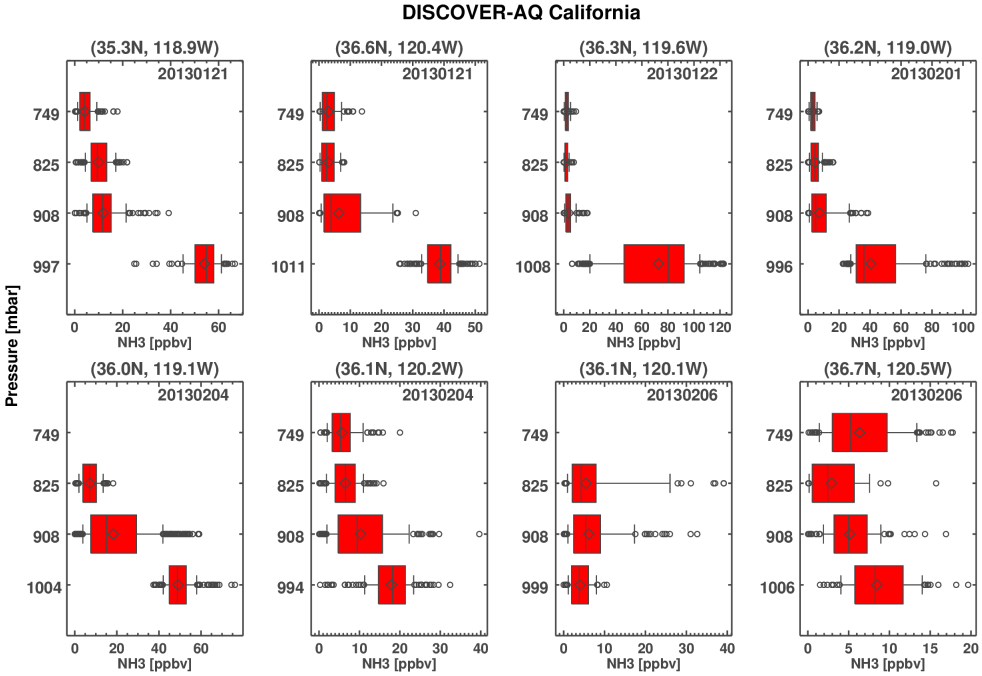

Figure S4: Statistics for the aircraft profiles corresponding to the retrieved CrIS profiles shown in S3. Rectangles denote the interquartile range (25% and 75%), whiskers the interdecile range (10% and 90%) and circles the outliers. The vertical bar corresponds to the median and the diamond the mean.

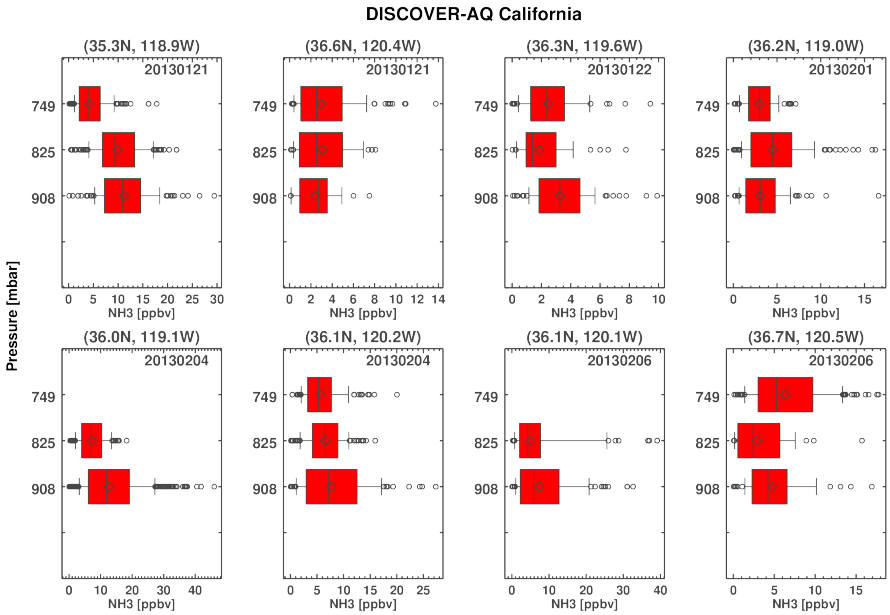

Figure S5: Same as S4, but with shortened range on the x-axis, for greater visibility of the range of measurements at higher altitudes.

Figure S5 zooms in on the aircraft data at and above the boundary layer, demonstrating the above the MLH most of the aircraft data are below the PTR-MS detectability level (7 ppbv) in California.