



*Supplement of*

## **Optimal estimation retrieval of tropospheric ammonia from the Geostationary Interferometric Infrared Sounder on board FengYun-4B**

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### Text S1. Comparison of NH<sub>3</sub> retrievals from two different micro-windows

The motivation of this comparison is to check the consistency of the retrieval results using two different micro-windows, which may have different spectral noise, as a way to check the robustness of the spectra observations. The micro-windows (920-940 cm<sup>-1</sup>) for NH<sub>3</sub> retrieval, to be compared with the micro-windows (955-975 cm<sup>-1</sup>) used in this study, is also originated from the NH<sub>3</sub>  $\nu_2$  rotational-vibrational transitions and shows similar absorption characteristics, as shown in **Figure S4**. Theoretically, applying the FY-GeoAIR algorithm using these two micro-windows should produce similar NH<sub>3</sub> retrievals. However, due to the impact of spectral noise, which is assumed to be close to random, the retrieval results are expected to show a discrepancy. In addition, the slight difference in their absorption structures and sensitivities, with micro-window #2 (i.e., 955-975 cm<sup>-1</sup>) presenting a stronger absorption and therefore higher sensitivity than micro-window #1 (i.e., 920-940 cm<sup>-1</sup>), may contribute to the discrepancy. As shown in **Figure S5(a)**, the DOFSs show high consistencies, with a correlation coefficient of 0.97, suggesting the two micro-windows contain similar information in capturing the NH<sub>3</sub> variabilities. We do observe a slightly higher DOFS for micro-window #2 resulting from its stronger absorption and sensitivity. In **Figure S5(b)**, the retrieved NH<sub>3</sub> columns are compared for retrievals with DOFS larger than 0.5, a threshold used to remove retrievals that gain weak constrain from the FY-4B/GIIRS spectra. The correlation coefficient between the two datasets is 0.82 with a root-mean-square-error of  $3.2 \times 10^{15}$  molec/cm<sup>2</sup>. Their agreement improves, with correlation coefficient of 0.86, when the data are filtered by DOFS > 0.7, as shown in **(c)**. The consistency, indicates that the small difference in absorption structure and sensitivity in the micro-windows are not causing large bias in the retrievals. The difference is primarily caused by spectral noise.

## **Text S2. The impact of a priori NH<sub>3</sub> vertical shape on the NH<sub>3</sub> retrievals**

Since the observation of infrared sounder is not equally sensitive to NH<sub>3</sub> abundance in every layer, setting an appropriate a priori NH<sub>3</sub> in the retrieval algorithm is important. Extra retrieval error may be introduced if the profile is far from the truth. This is because the perturbation by the observed spectra on the sensitive layers may propagate into other layers with less sensitivity. Previous study by **Whitburn et al. (2016)** has shown that the difference in the a priori NH<sub>3</sub> profile is not causing significant bias in retrievals using polar orbiting satellite retrievals. Here we carried out a simple experiment to examine the impact of different vertical shape of a priori NH<sub>3</sub> on the retrieved columns. The a priori profiles used in the retrieval algorithm are generated by perturbing the PBL portions of the a priori, where NH<sub>3</sub> is concentrated, used in FY-4B/GIIRS by 2 and 0.5 times, respectively, as shown in **Figure S6(a)**. These perturbed profiles are uniformly scaled so that the total columns equal to the original a priori column. We used these profiles for the retrieval on the six representative days, as in the synthetic experiment described in **Section 3.5**, in the North China Plain. The retrievals based on perturbed profiles are then compared with original retrievals, shown in **Figure S6(b)** and **(c)**. In general, we see that the results using the reduced PBL excess profile have smaller values while the results using the enhanced PBL excess profile show larger values than the original retrievals. The results show that the mean and standard deviation of the fractional error are 1.0% and 9.65%, respectively, for the reduced PBL excess profile, and 0.9% and 7.6%, respectively, for the enhanced PBL excess profile. The absolute root-mean-square errors for both cases are about the same  $3.4 \times 10^{15}$  molec/cm<sup>2</sup>. Fortunately, there are no large systematic bias and the averaged error is within 10% in our cases of profiles differ by a factor of 2.

Figure S1. Histograms of (top) the reduced  $\chi^2$  and (bottom) the root-mean-square-error (RMSE) of the fitting residual.

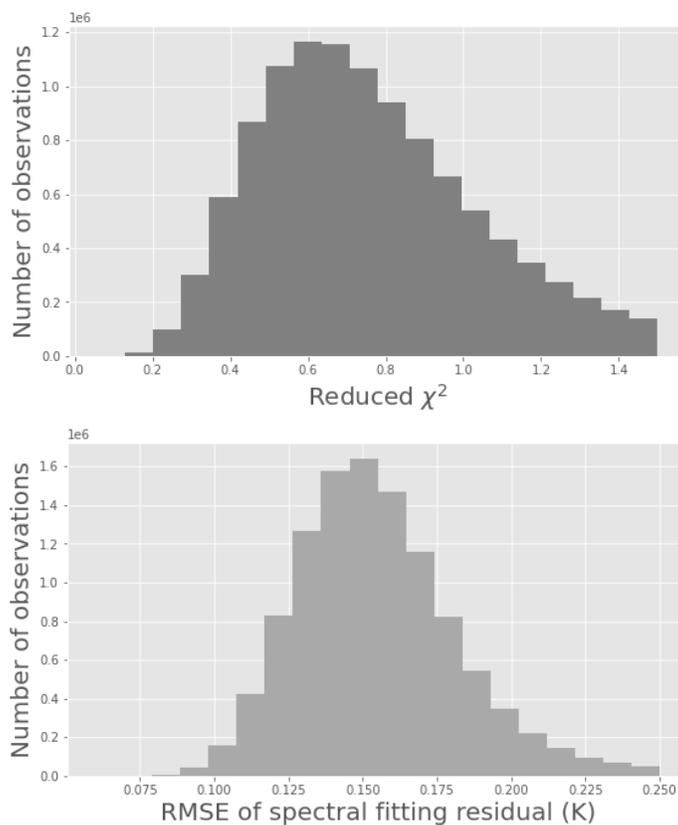


Figure S2. Similar to Figure S1, but for retrievals before applying the data filtering as described in Section 3.4.

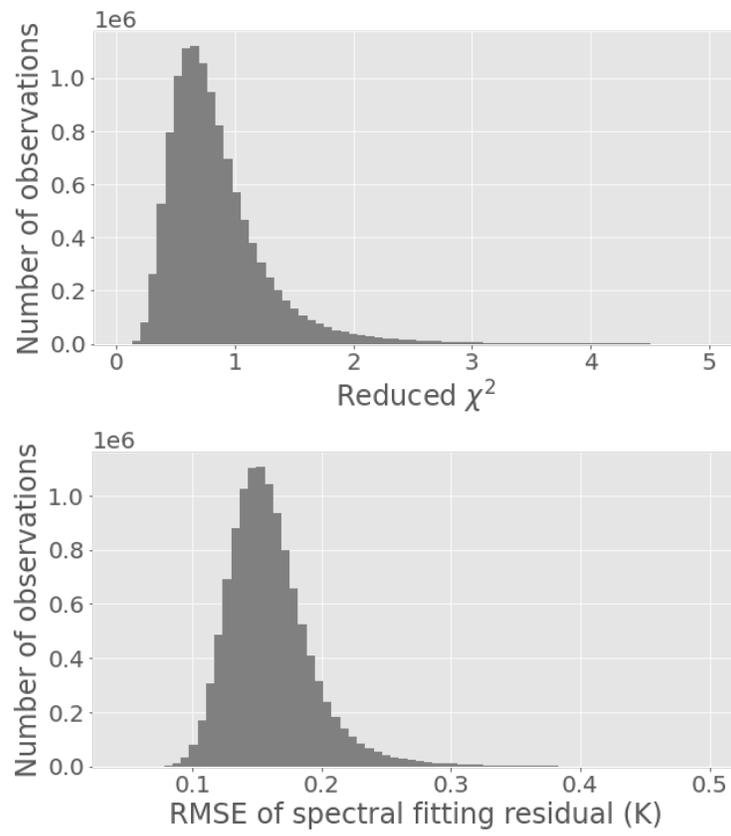


Figure S3. Spatial maps of TC averaged in July (summer), October (autumn), and December (winter), respectively, using 2-3h, 8-9h, 14-15h, and 20-21h in Beijing Time (BJT) to represent mid-night, early morning, afternoon, and early evening, respectively.

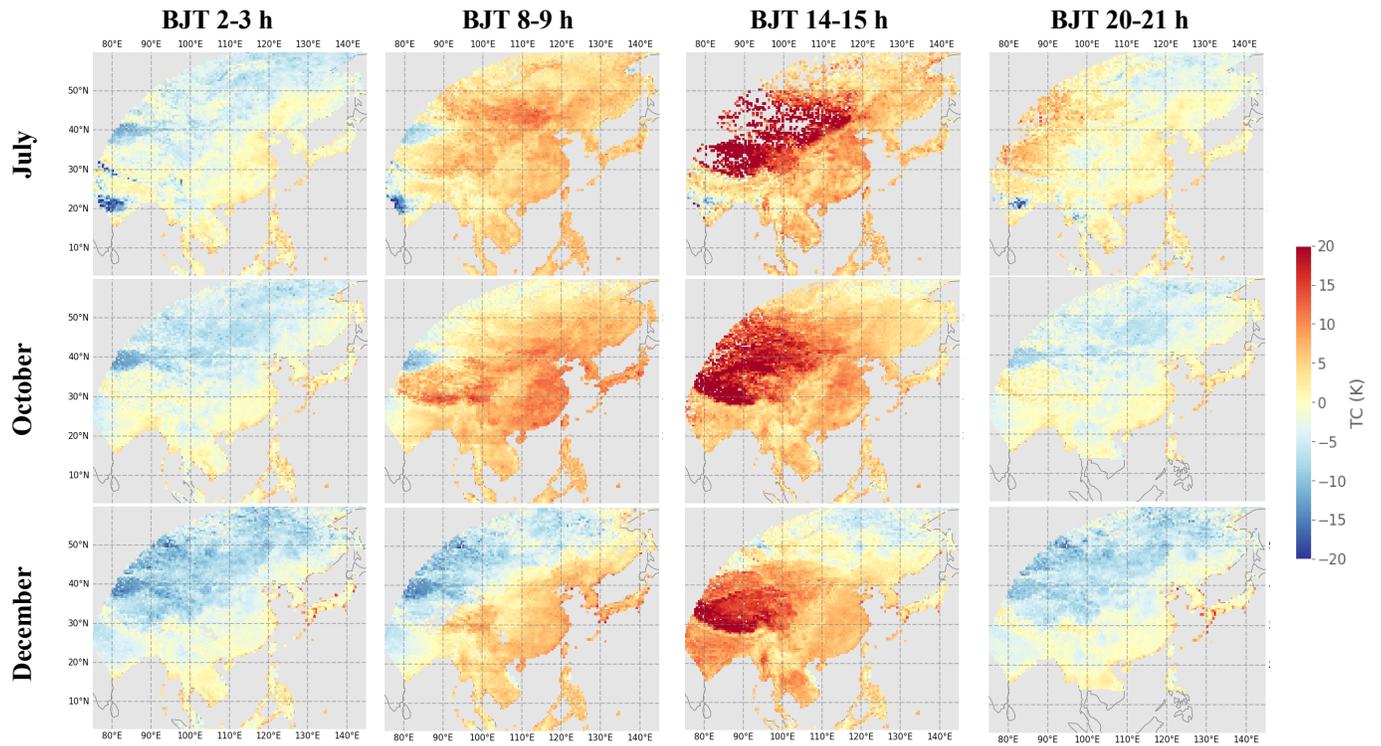
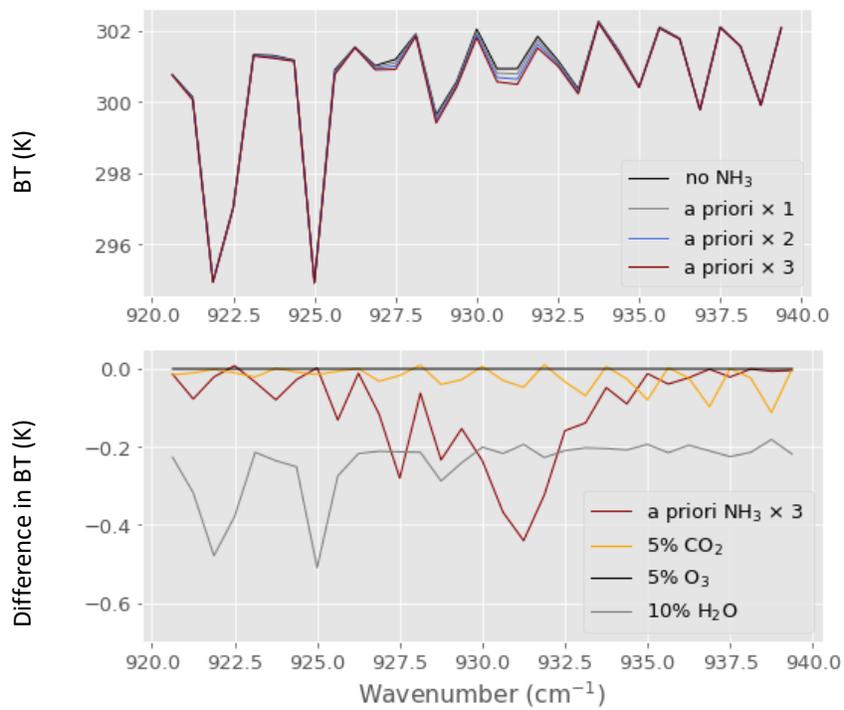
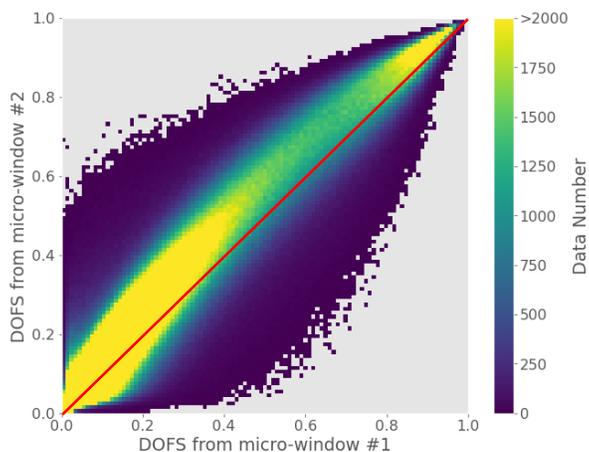


Figure S4. Sensitivity experiment comparing absorptions of NH<sub>3</sub>, CO<sub>2</sub>, O<sub>3</sub> and H<sub>2</sub>O in the micro-window, similar to Figure 2, but for the 920-940 cm<sup>-1</sup> micro-window.

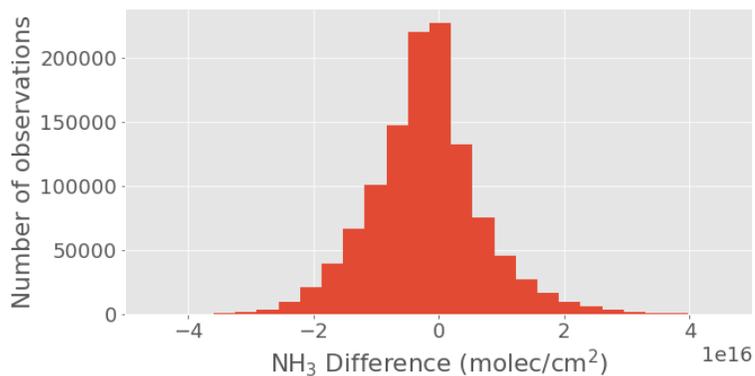
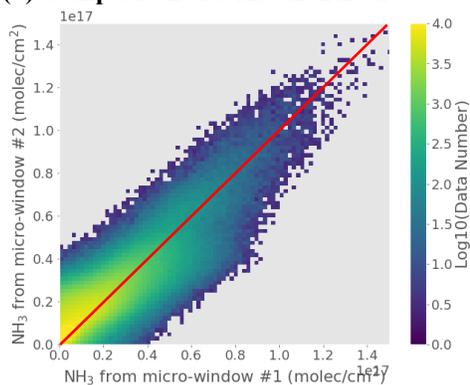


**Figure S5. Comparison of NH<sub>3</sub> retrievals using micro-window #1 (920-940 cm<sup>-1</sup>) and micro-window #2 (955-975 cm<sup>-1</sup>): (a) the DOFS, which shows a correlation coefficient of 0.97 for a total of 11.7 million data points; (b) the retrieved NH<sub>3</sub> columns filtered by DOFS>0.5. For the comparison of columns, in total, 1.1 million data points are available. The correlation coefficient between the two column datasets is 0.82 with a root-mean-square-error of  $9.2 \times 10^{15}$  molec/cm<sup>2</sup>. The histogram is also shown; (c) the retrieved NH<sub>3</sub> columns filtered by DOFS>0.7. In total, 0.5 million data points are available for comparison. The correlation coefficient is 0.86 with a root-mean-square-error of  $8.6 \times 10^{15}$  molec/cm<sup>2</sup>. The mean errors are  $2.0 \times 10^{15}$  and  $2.7 \times 10^{15}$  molec/cm<sup>2</sup>, respectively, for (b) and (c).**

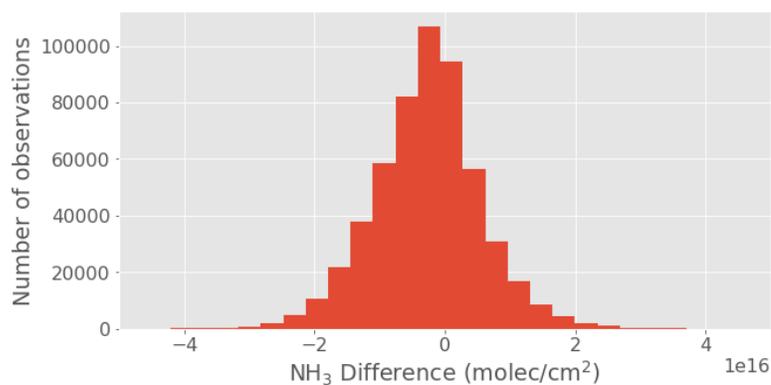
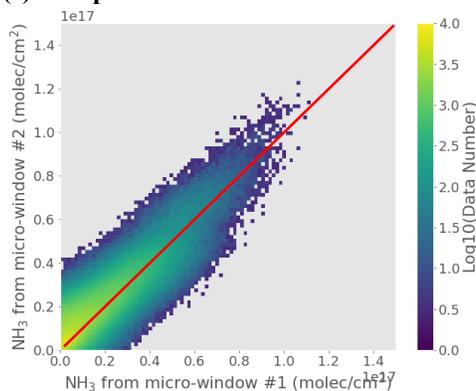
**(a) Comparison of DOFS**



**(b) Comparison of NH<sub>3</sub> when DOFS>0.5**



**(c) Comparison of NH<sub>3</sub> when DOFS>0.7**



**Figure S6. Comparison of retrieval results of NH<sub>3</sub> columns using different a priori NH<sub>3</sub> profiles. (a) The NH<sub>3</sub> a priori profile with reduced PBL excess by 50% and enhanced PBL excess by 2 times; (b) The comparison of the retrieved NH<sub>3</sub> column using the reduced PBL excess profile. The mean of the fractional error is 1.0% while the standard deviation is 9.6%; (c) The comparison of retrieved NH<sub>3</sub> column with enhanced PBL excess profile. The mean of the fractional error is 0.9% and the standard deviation is 7.6%. The green lines are the 1:1 line in (b) and (c).**

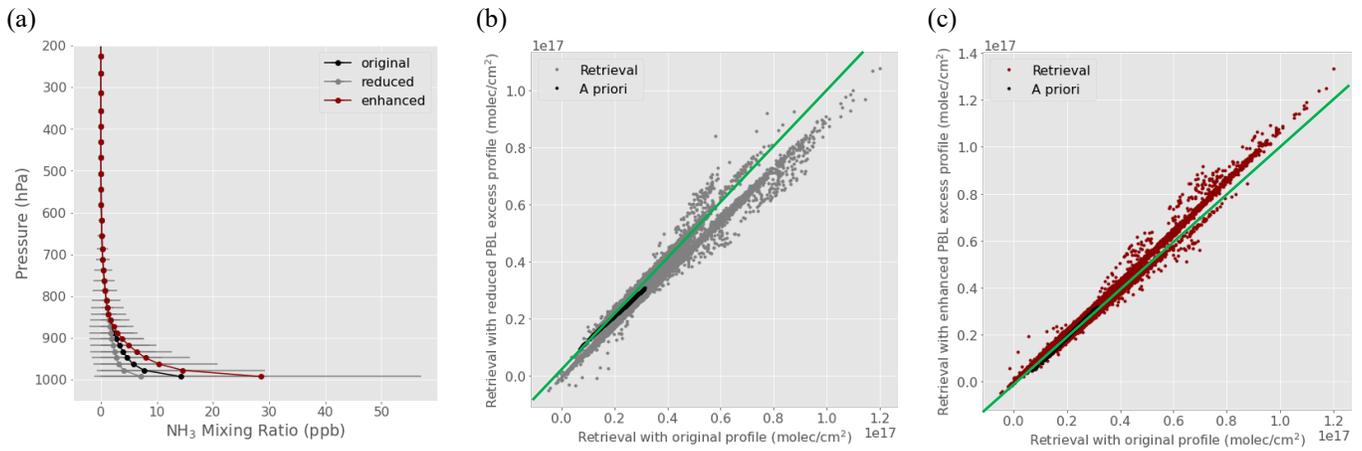


Figure S7. Observation hours (in Beijing Time) of IASI NH<sub>3</sub> retrievals in (a) the daytime on July 07, 2022, and (b) the nighttime on December 18, 2022.

