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Supplement of

Performance of AIRS ozone retrieval over the central Himalayas: use of ozonesonde and other satellite datasets

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S1. Methodology

S1.1 Methods of Analysis

First, ozonesonde data were interpolated at all AIRS Radiative Transfer Algorithm (RTA) layers from surface to burst altitude, then ozonesonde profiles were smoothed according to the AIRS averaging kernel and a-priori profile (ML climatology), leading to a vertical profile [ozonesonde (AK)] representing what AIRS would have measured for the same ozonesonde sampled atmospheric air mass in the absence of any other error affecting satellite observations. According to Rodgers and Connor (2003), the smoothing of the true state can be characterized as follows:

$$X_{est} = X_0 + A' (X_{sonde} - X_0) \qquad \text{(S1)}$$

The AIRS provides averaging kernels information at 9 pressure levels (Figure 2b) whereas the AIRS RTA has 100 pressure levels. So following ozone vertices (Table S3) and formulating trapezoid matrix (Figure 2a, the details regarding the calculation of trapezoid matrices are given in AIRS/AMSU/HSB Version 6 Level 2 Product Levels, Layers and Trapezoids), we convert 9 levels AIRS averaging kernels to 100 levels averaging kernels using following defined operation.

$$A' = F \times A_{trapezoid} \times F' \qquad \text{(S2)}$$

Where $A_{trapezoid}$ and F are averaging kernel matrices and trapezoid matrices (F' is pseudo-inverse of F). $A_{trapezoid}$ is a given product, while F is calculated for given ozone vertices (Table S3).

Further, in the thermal IR spectrum, the contribution of ozone or any other trace gas towards emission/absorption of IR radiation in the radiative transfer equation depends on the exponent of layer integrated column amounts (Maddy and Barnet, 2008). Hence logarithmic changes in layer column density are more linear than absolute changes. So logarithmic equations are used instead of Eq. S1 for smoothing ozonesonde data in the present study.

S1.2 Statistical Analysis

The error analysis for AIRS retrieval with interpolated and smoothed ozonesonde is based on Nalli et al. (2013, 2017). Bias, root mean squared error (RMSE), and standard deviation (STD) are studied at various RTA vertical levels from the surface to 10hPa over the Himalayan region. The finer spatio-temporal collocation utilized here has further minimized the uncertainty and error in the evaluation. Since the observation site (29.4^o N, 79.5^o E) is at a latitude lower than 45^o; hence there is a lesser overlap of satellite passes, and mostly a few nadir scans are close to the observation site (mostly daytime granules in the range of 75 to 85). Hence all the daytime observations of AIRS are close to ± 3 hours of temporal collocation to the ozonesonde launch and possess a lesser chance of time mismatch.

Given the collocated ozone mixing ratio profiles for satellite, ozonesonde (AK), and in-situ truth (ozonesonde) observations, the statistical errors are calculated as follows -

$$\text{RMSE}\ (\Delta O_l) = \sqrt{\frac{\sum_{j=1}^{j=n} W_{l,j} \times (\Delta O_{l,j})^2}{\sum_{j=1}^{j=n} W_{l,j}}} \qquad \text{(S4)}$$

$$\text{Bias}\ (\Delta O_l) = \frac{\sum_{j=1}^{j=n} W_{l,j} \times (\Delta O_{l,j})}{\sum_{j=1}^{j=n} W_{l,j}} \qquad \text{(S5)}$$

Here l runs over different RTA layers and j runs for all collocated profiles, $\Delta O_{l,j}$ the fractional deviation is taken to be the absolute deviation divided by the observed value. Where $\Delta O_{l,j}$ = $\left(\frac{O^R{}_{l,j} - O^T{}_{l,j}}{O^T{}_{l,j}}\right)$, O^T and O^R are ozonesonde/ozonesonde (AK) and satellite retrieved ozone mixing ratio, respectively. $W_{l,j}$ is the weighting factor and assumes one of three forms $W_0 = 1$, $W_1 = O^R$ and $W_2 = (O^R)^2$ and for ozone to minimize skewing impact due to large variation in mixing ratio at different altitudes, we have used the W_2 weight factor as suggested by other sounder science team (Nalli et al., 2013, 2017). The Standard deviation (STD) is then calculated by the square root of difference between RMSE and biases square at different RTA levels. Further to check the strength of the linear relationship between the satellites retrieved data and ozonesonde data the square of Pearson's correlation coefficient is also calculated.

S1.3 Estimation of Columnar Ozone

The total column ozone (TCO) from ozonesonde is calculated by integrating the ozone mixing ratio from the surface to burst altitude and then adding residual ozone above burst altitude. Here the residual ozone is obtained from satellite-derived balloon-burst climatology (BBC) (McPeters and Labow, 2012; Stauffer et al., 2022). The discrete integration for calculation of total ozone column (DU) between defined boundaries is performed as follows:

$$\text{Total column ozone} = 10^7 \times \left(\frac{RT_o}{g_o P_o}\right) \times \sum_{j=1}^{j=n} 0.5 \times (VMR[i] + VMR[i+1]) \times (P[i] - P[i+1]) \quad \text{(S6)}$$

Where P is ambient pressure in hPa, VMR volume mixing ratio of ozone in ppbv, R (= 287.3 $JKg^{-1}K^{-1}$) gas constant, g_o (= 9.88 ms^{-2}), P_o (= 1.01325×10^5 Pa) and T_o (= 273.1 K) standard temperature.

The UTLS ozone column (DU) is also calculated using Eq. (S6), where the UTLS region is defined between 400 hPa to 70 hPa (Bian et al., 2007). Additionally, the tropospheric ozone column (DU) is calculated for ozonesonde utilizing Eq. (S6) with boundaries from the surface to the lapse rate tropopause (LRT). The tropopause height from balloon-borne observations is estimated using the lapse rate method as well as the AIRS-derived tropopause is used and shown in Figure 3. However, for OMI and MLS tropospheric ozone residual method is used, which calculates the tropospheric ozone column by subtracting the OMI total column from MLS stratospheric ozone column (Hudson et al., 1998; Ziemke et al., 2006).

Supplementary Tables

Table S1. AIRS means DOF as calculated for different atmospheres for version 5 (Maddy and Barnet, 2008).

Retrieved Quantity	Tropical	Mid-latitude	Polar
Temperature	6.67	6.40	5.65
Water Vapour	4.46	3.85	2.89
Ozone	1.36	1.64	1.66
Carbon monoxide	0.78	0.84	0.65
Methane	1.06	0.94	0.70

Table S2. Quality Control for NOAA/CLASS data sets (QC 2 and 4 are obsolete).

AWIPS Dot Color	**EDR Quality Flag**	**Meaning**
Green	0	Clear Sky/Partly Clear Conditions Successful infrared (IR) + microwave (MW) retrieval.
Yellow	1, 16, or 17	Cloudy Conditions Failed IR+MW retrieval. Successful MW-only retrieval
Red	9 or 25	Precipitating Conditions Failed IR+MW retrieval. Failed MW-only retrieval.

Table S3. Typical ozone vertices used to calculate the trapezoid and averaging kernels.

Press. (hPa)	0.0160639	20.9224	51.5277	71.5397	103.017	142.385	212.028	300.000	596.306	1100.00
Index	1	26	35	39	44	49	56	63	80	100

Table S4. Coefficient of determination between AIRS and ozonesonde. Tropospheric ozone column is estimated using AIRS tropopause.

	Total Ozone Column	UTLS Ozone Column	Tropospheric Ozone Column
AIRS Vs ozonesonde	0.50	0.75	0.72

Table S5. UTLS ozone column difference between AIRS, MLS, and ozonesonde.

UTLS Difference (DU)	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
AIRS – MLS	6.1	6.3	7.1	16.0	18.5	16.7	10.9	8.5	7.8	8.1	8.1	8.9
AIRS -ozonesonde	6.2	9.8	11.9	9.5	11.7	8.6	6.9	3.6	3.1	3.5	7.7	4.7

Supplementary Figures

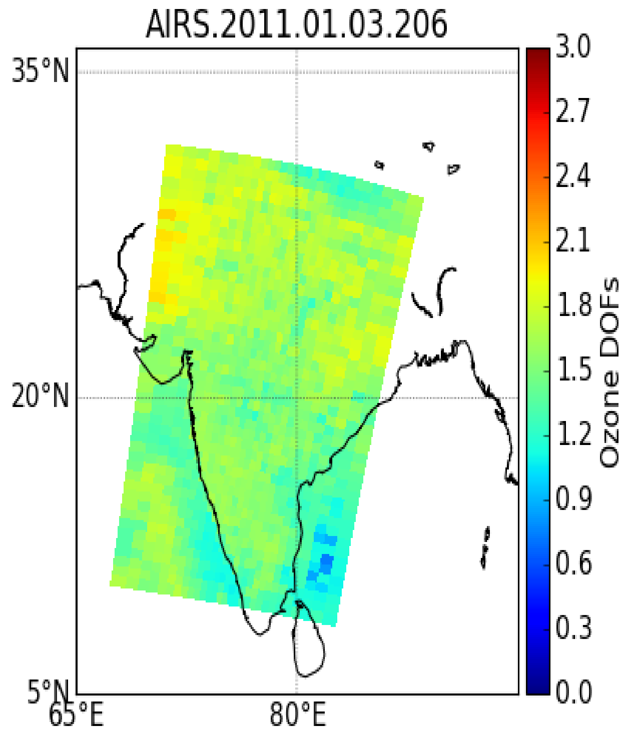

Figure S1. Spatial distribution of degree of freedoms (DOFs) of AIRS retrieved ozone for 3 January 2011 over India.

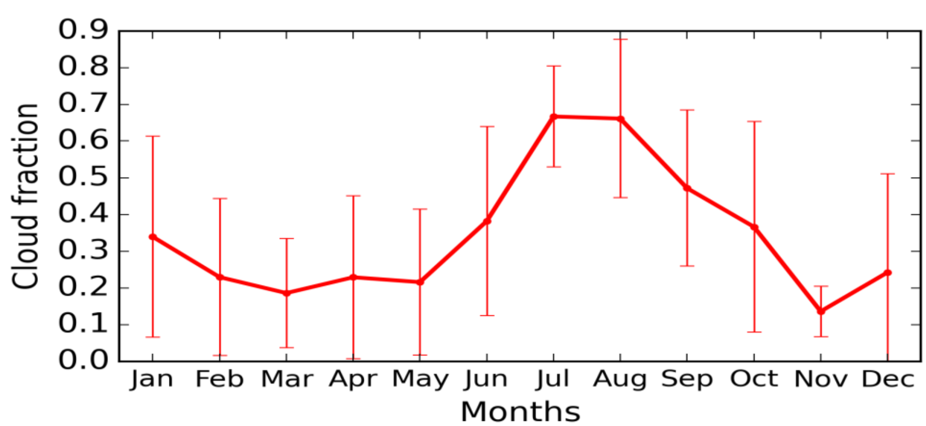

Figure S2. Total cloud fraction over the observation site as seen by AIRS for different months.

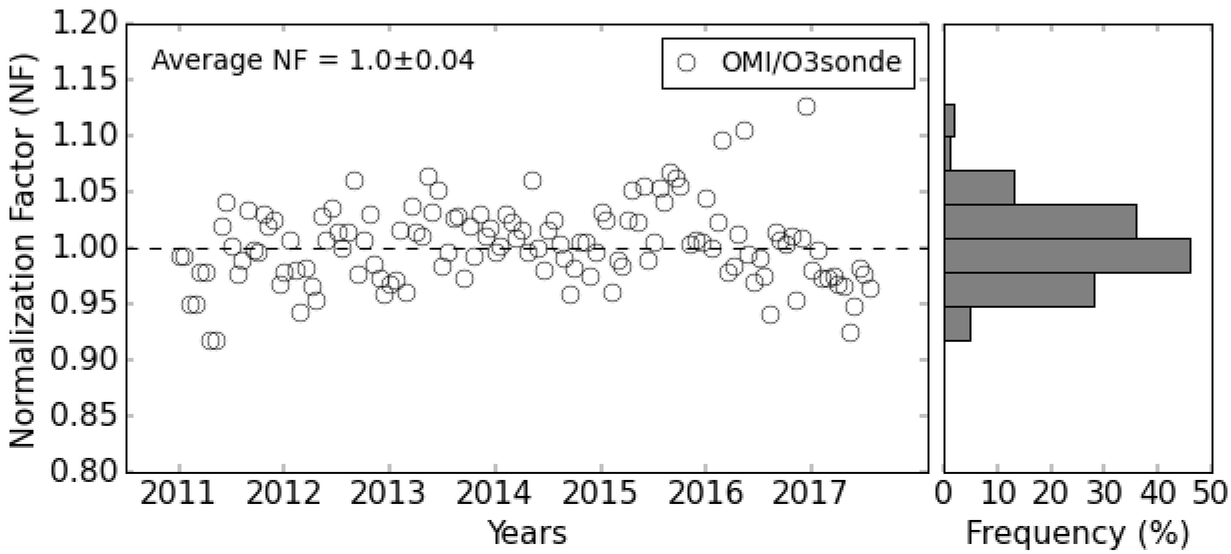

Figure S3. Estimated total ozone normalization factor of ECC ozonesonde with the Aura OMI satellite instrument. Corresponding frequency histograms are also shown on the right.

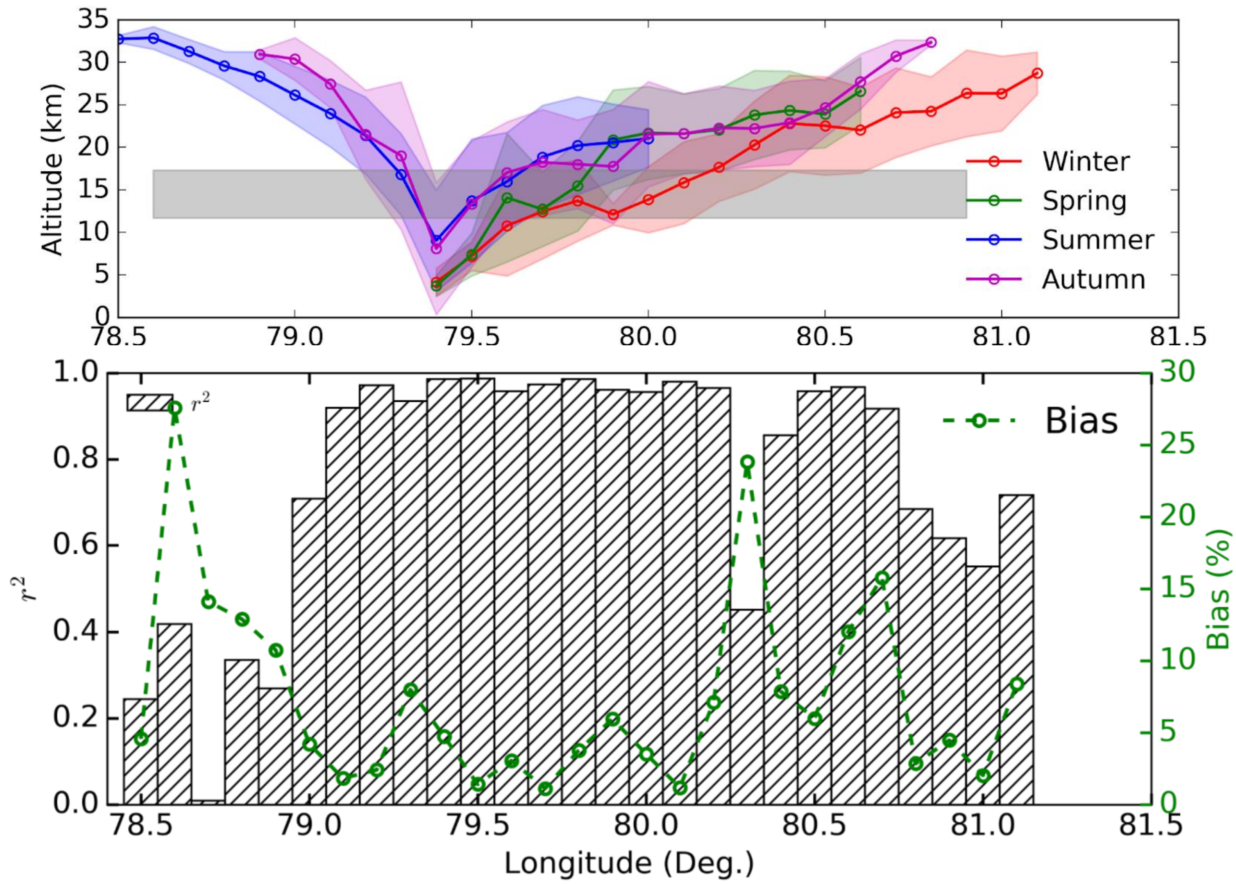

Figure S4. (a) Altitude variations of the balloons along longitudes during four seasons. The one sigma spread is also shown with a shaded area. The rectangle grey shaded area shows the tropopause region (mean ± sigma) from ozonesonde over Nainital. Nainital longitude is 79.45^{o}E. (b) The bottom panel shows the longitudinal variations in r^2 (coefficient of determination) and biases between ozonesonde and AIRS retrieved ozone.

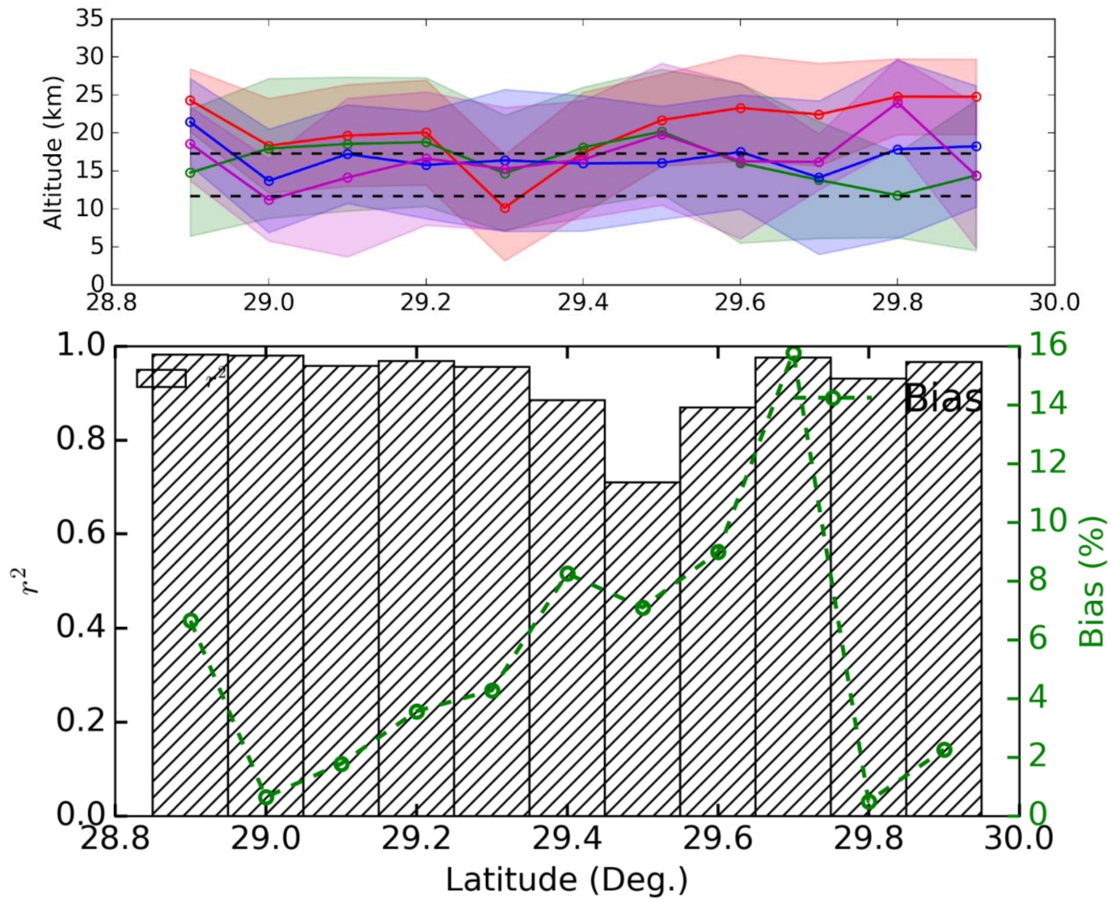

Figure S5. Altitude variations of the balloons along latitudes during four seasons. The one sigma spread is also shown with a shaded area. The area between the black dash lines shows the tropopause region (mean ± sigma) from ozonesonde over Nainital. The bottom panel shows the variation of r^2 (coefficient of determination) and biases between ozonesonde and AIRS retrieved ozone concentration along the latitude.

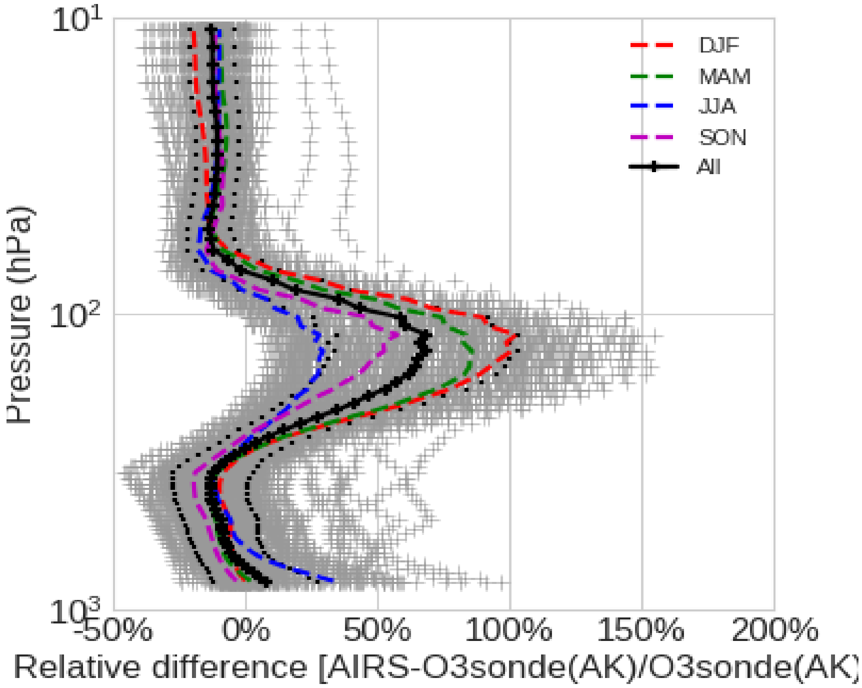

Figure S6. The relative difference of AIRS and ozonesonde(AK) for 2011-2017. Individual profiles are shown by a plus sign and dashed line for the average profile.

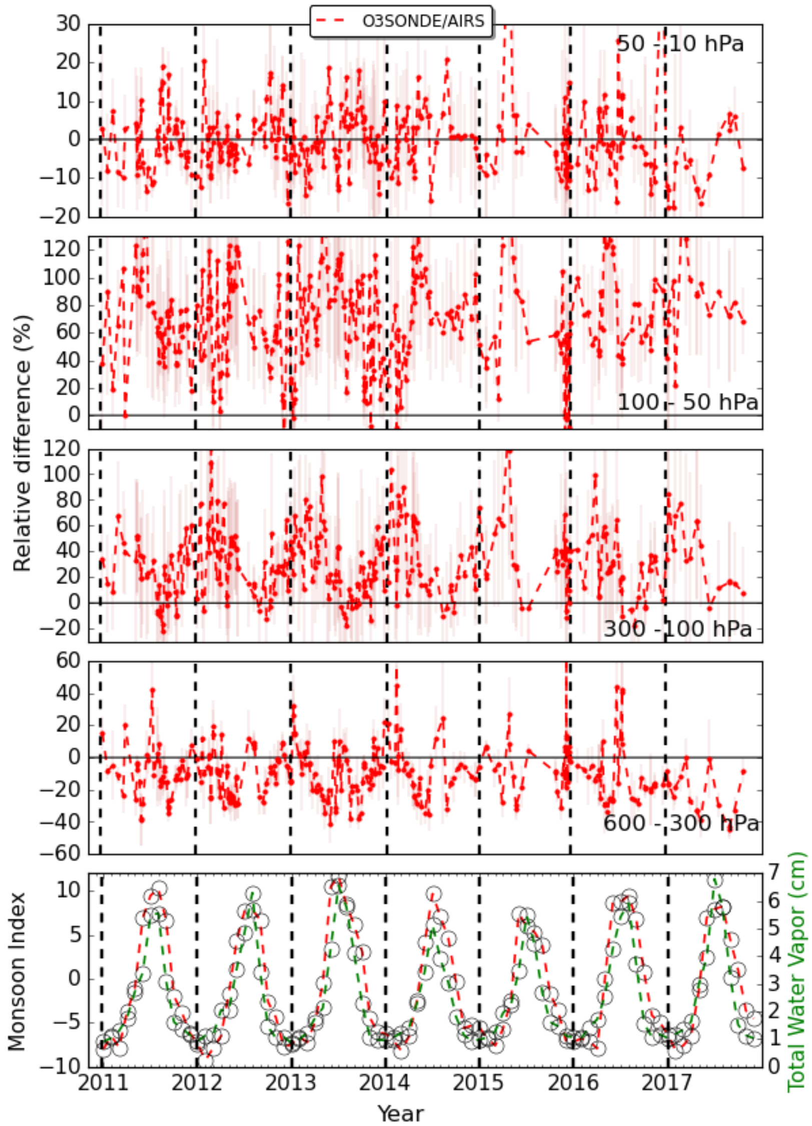

Figure S7. Partial ozone column difference (%) time series for seven years at three defined layers, characterizing the middle stratosphere (50 - 10 hPa), the lower stratosphere (100 – 50 hPa), the upper troposphere (300 - 100 hPa), the middle troposphere (600 - 300 hPa), respectively. The percentage difference is calculated as [(AIRS-Ref_O3)/Ref_O3]*100, where Ref_O3 is ozonesonde and ozonesonde (AK). The monthly variation of the Indian monsoon index and total water vapor is also shown at the bottom.

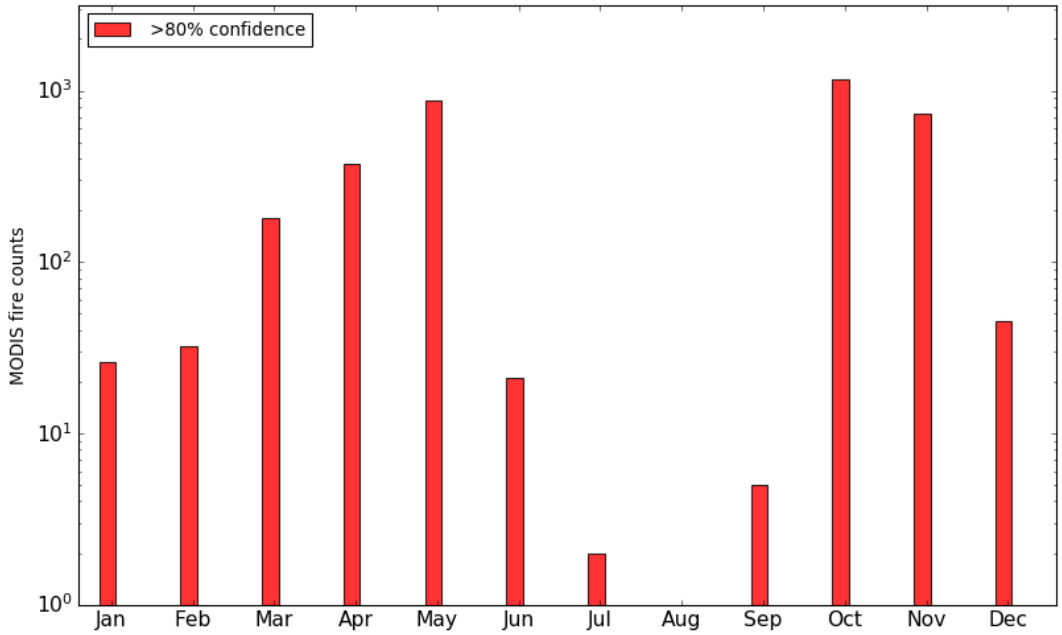

Figure S8. Monthly variation (2011-2017) of MODIS fire counts (>80% confidence) over northern India.

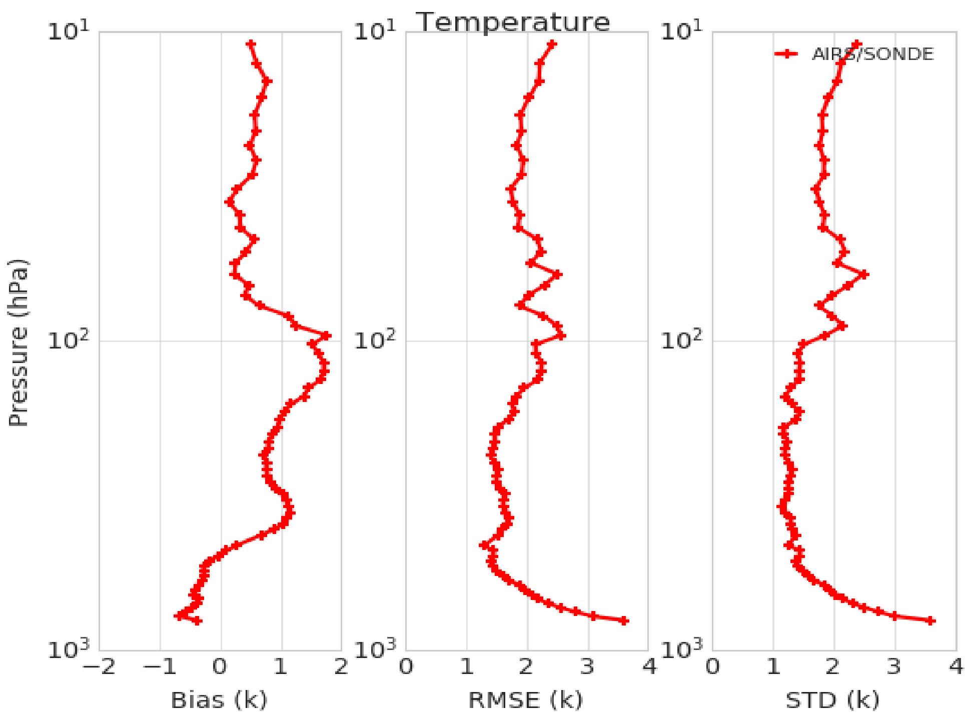

Figure S9. Statistical error analysis of AIRS temperature retrieval with interpolated balloon-borne observations for seven years (2011 – 2017).

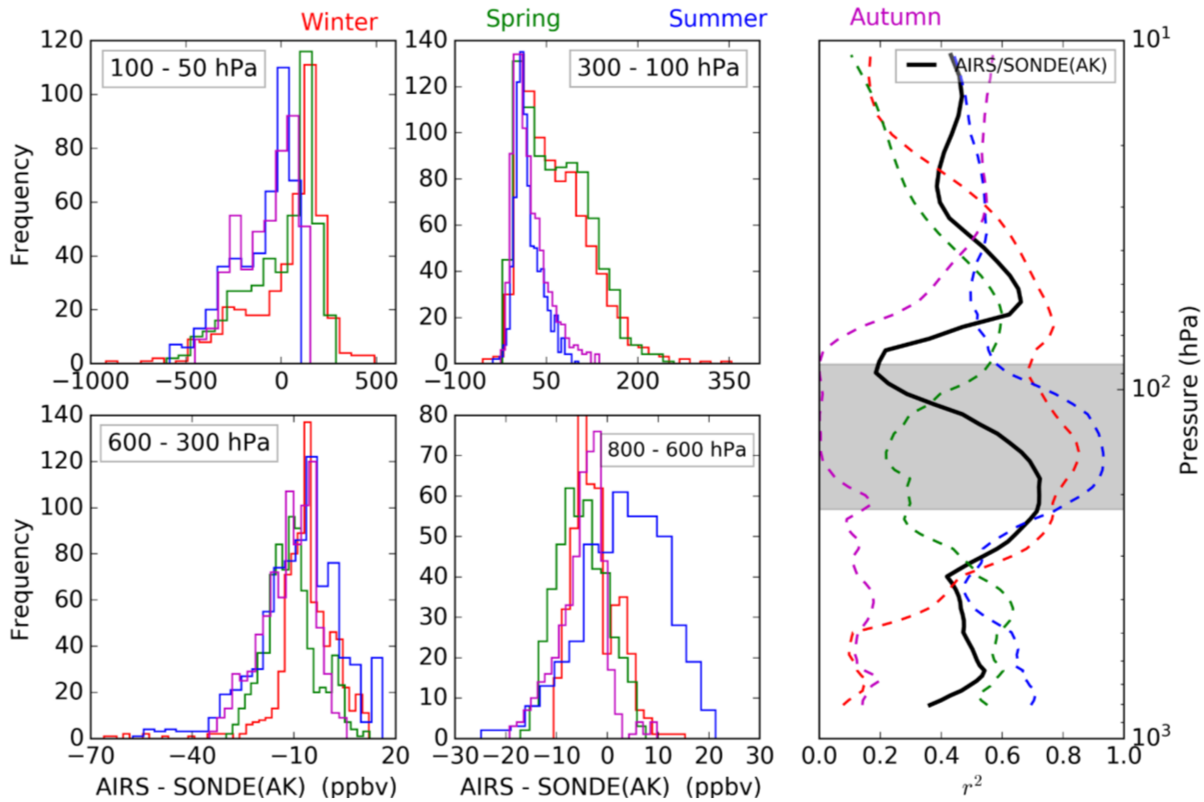

Figure S10. Histogram difference between AIRS ozone and ozonesonde (AK) in the four defined layers. The average correlation profiles between AIRS ozone and ozonesonde (AK) are shown on the right during winter (red), spring (green), summer-monsoon (blue), and autumn (magenta). The black line is for the entire data set. The grey shaded area shows the tropopause region from balloon-borne radiosondes observations.

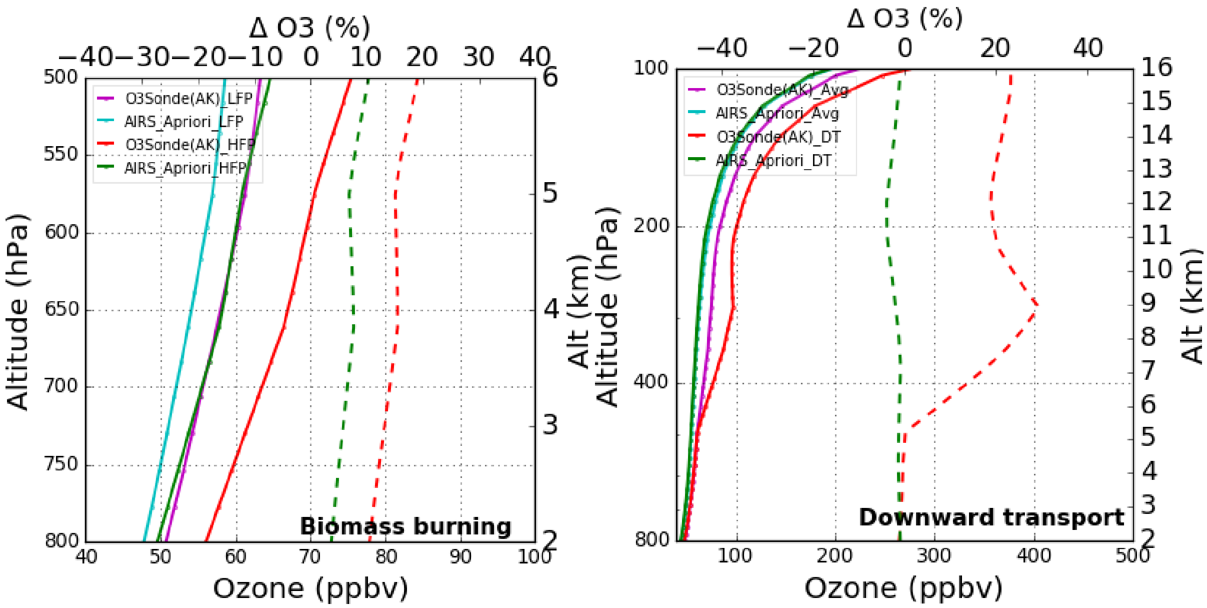

Figure S11. Biomass burning (BB) and downward transport (DT) profile for AIRS a-priori (or first guess) and ozonesonde data. The solid line corresponds to ozone profiles while the dotted line shows a % increase in ozonesonde (red) and AIRS a-priori (green) profile in BB and DT influence.