Supplement of Atmos. Meas. Tech., 18, 5749–5762, 2025
https://doi.org/10.5194/amt-18-5749-2025-supplement

Atmospheric Measurement Techniques
Open Access

Supplement of

Feasibility of a space-borne terahertz heterodyne spectrometer for atomic oxygen and temperature in the mesosphere and lower thermosphere

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S1 Convergence During Retrieval

In the retrieval process, the parameters describing temperature, atomic oxygen concentration, and spectral shifts are estimated using the iterative Gauss-Newton method. In this approach, the forward problem, i.e. simulating the spectra used for the given retrieval, is linearised around the current estimates of these parameters. We do that using the forward difference method. The resulting linearisation allows the parameters to be updated through a linear least-squares solution yielding improved estimates. For the least-squares solution, we use the function *lsq_linear* from the *scipy* library. To avoid oscillations of the parameter estimates around the minimum, we update the parameters as an weighted average between the newly found least-squares solution and the parameters in the previous iteration such that

$$\vec{x}_{i+1} = 0.6 \cdot \vec{x}_{i+1}^{lsq\_linear} + 0.4 \cdot \vec{x}_i \ , \tag{S1}$$

where $\vec{x}_{i+1}$ is the vector containing the improved parameter estimates, $\vec{x}_i$ is the vector containing the parameter estimates in the previous iteration, and $\vec{x}_{i+1}^{lsq\_linear}$ is the parameter estimates from the least squares solution. We stop the iterative process when the temperature and atomic oxygen parameters change less than 10^{-3}, the sum of all the shifts less than 10 kHz, and the residuals, relative to the residuals in the previous step, change less than 10^{-6}. Figure S1 shows the parameter values during the retrieval from combining scan 14,15,16, where convergence occurs within 15 iterations. The convergence behavior for the remaining retrievals is similar and is therefore not shown.

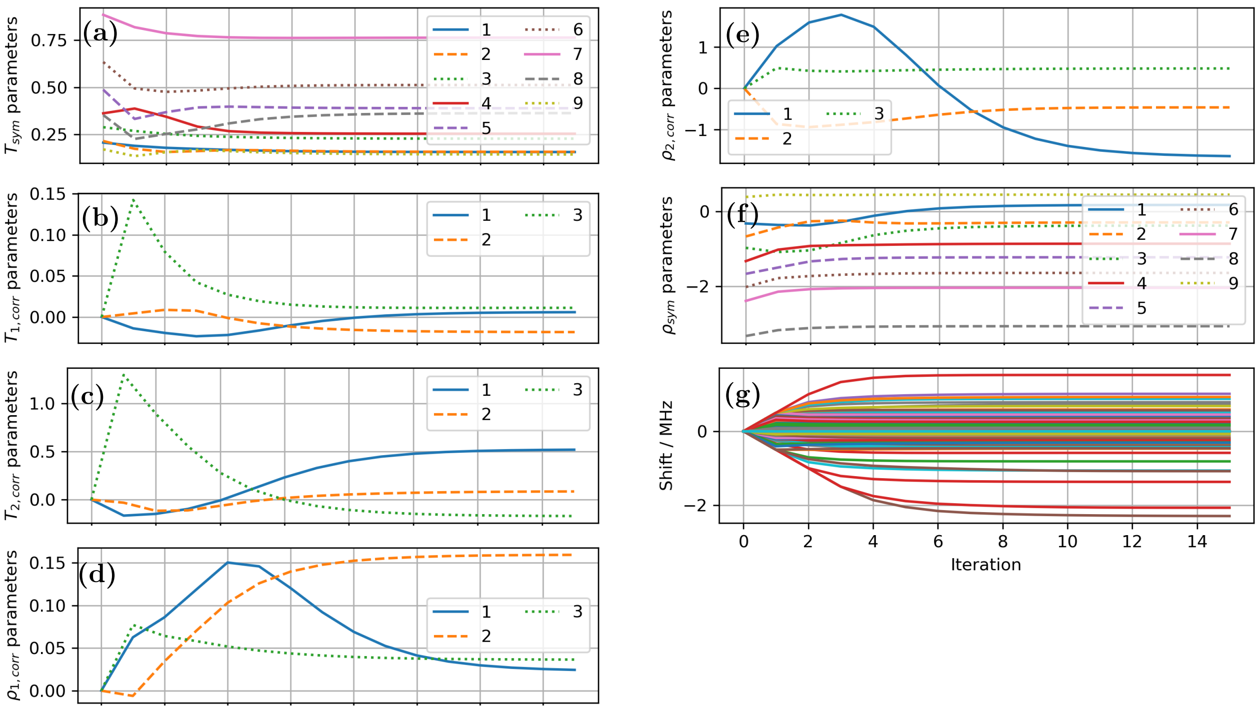

Figure S1: *Parameter values at each iteration in the Gauss Newton method for the retrieval at the 14th combined scan (scan 14,15,16).* ***(a, b, c)*** *Parameters of the temperature parametrisation.* ***(d, e, f)*** *Parameters of the atomic oxygen parametrisation.* ***(g)*** *The parameters for the shifts. The parameters have been scaled/shifted upon retrieval for obtaining values of around ±1. For T_{sym} and ρ_{sym}, parameter numbers from 1 to 6 and 1 to 7, respectively, corresponds to the B-spline coefficients, in increasing altitude order. For an example, the B-spline coefficient for T_{sym} are scaled by 10^{-3}. The shifts are scaled by 10^{-6} (scaled to MHz). Due to the many parameters, the shift's parameters are not numbered.*

S2 Single Scan Retrievals Versus Combined Scan Retrievals

To assess the significance of the second-order correction for spherical asymmetry, retrievals using single scans without any correction were also performed. Figure S2 shows the resulting mean deviations in temperature and atomic oxygen concentrations versus altitude, comparing them to the deviations from retrievals using combined scans with the second-order correction applied (Figure 17 in manuscript). The deviations from the single scans are significantly larger. For an example, at an altitude of 110 km, the single-scan deviations are approximately five times larger. This exceeds the expected factor of square-root three, which would result solely from the increased signal provided by combining three scans. These results demonstrate that applying spherical asymmetry corrections is essential for achieving accurate retrievals for the proposed mission scenario.

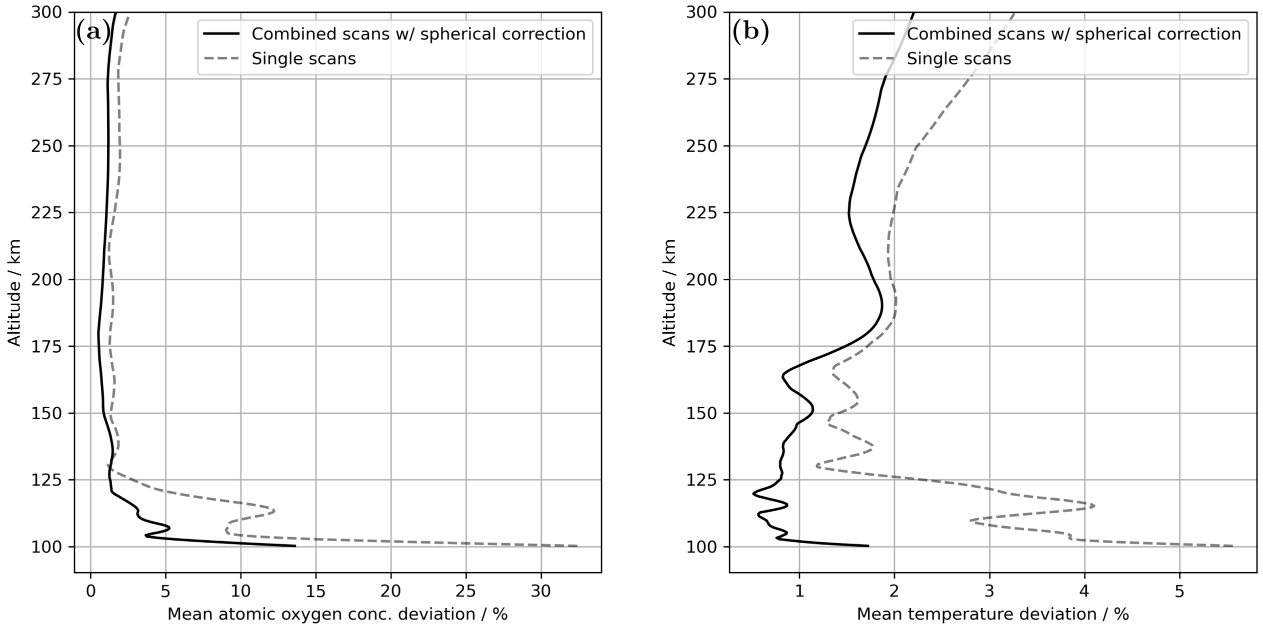

Figure S2: *Average deviations for all the retrieved temperature and atomic oxygen concentration vertical profiles. Dashed grey line showing the average deviations from single scan retrievals and black solid line showing the average deviations from combined scans with second order correction for spherical asymmetry.* ***(a)*** *Temperature deviations.* ***(b)*** *Atomic oxygen concentration deviations.*