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Assessment of water vapor isotopologue measurements by ACE-FTS and Odin-SMR

Ralf Bauer (1), Patrick Sheese (1), Kaley Walker (1,2), Joachim Urban (3), Donal Murtagh (3), Chris Boone (2), Peter Bernath (4,5), Gloria Manney (6,7)

(1) University of Toronto, Toronto, Canada (rbauer@atmosp.physics.utoronto.ca), (2) University of Waterloo, Waterloo, Canada, (3) Chalmers University of Technology, Gothenburg, Sweden, (4) Old Dominion University, Norfolk, USA, (5) University of York, York, UK, (6) NorthWest Research Associates, Redmond, USA, (7) New Mexico Institute of Mining and Technology, Socorro, USA

Knowing the isotopic composition of trace gases can improve our understanding of processes in the Earth's atmosphere causing isotopic fractionation. In many studies, isotopologue (molecules of identical chemical but different isotopic composition) amounts are primarily discussed as δ values, which are defined relative to a standard, e.g.:

$$\delta^{18}O(\%) = \left(\frac{(VMR_{H_2^{18}O}/VMR_{H_2^{16}O})}{(VMR_{H_2^{18}O}/VMR_{H_2^{16}O})_{VSMOW}} - 1\right) * 1000 \tag{1}$$

with VSMOW as Vienna Standard Mean Ocean Water. This study targets the water vapor isotopologues $H_2^{18}O$ and $H_2^{17}O$ in the stratosphere and lower mesosphere using $\delta^{18}O$ and $\delta^{17}O$ for the comparison.

Over the past decades, $H_2^{18}O$ and $H_2^{17}O$ profiles have been measured with balloon-borne (e.g. FIRS-2, Mk IV) and space-borne (e.g. ATMOS/SL3) instruments. The satellite instruments ACE-FTS (Atmospheric Chemistry Experiment - Fourier Transform Spectrometer) on the Canadian satellite SCISAT and SMR (Sub-Millimetre Radiometer) on the Swedish satellite Odin provide a significantly larger number of individual profiles with global coverage. Both instruments are still operational and provide data products for more than 10 years. Assessing their data quality is of key importance before conclusions can be drawn from these results.

ACE-FTS on SCISAT is an infrared Fourier Transform Spectrometer with a high spectral resolution of 0.02 cm⁻¹ and a spectral range from 750 to 4400 cm⁻¹. It measures using solar occultation viewing geometry. SCISAT is in a high inclination orbit at an altitude of 650 km. It was launched in August 2003 and has been performing routine measurements since February 2004.

SMR on Odin measures millimetre wave emissions from the atmosphere with a 1.1 m telescope in the 486 to 581 GHz range with four tunable radiometers. Odin was launched in February 2001 into a quasi-polar sunsynchronous orbit at about 600 km altitude. Spectral regions for the target trace gases are selected for SMR using different measurement modes and thus not all retrieved species can be measured simultaneously.

In order to perform the comparison between ACE-FTS and SMR $\rm H_2^{18}O$ (using $\delta^{18}O$), a maximum temporal difference of 5 hours and a maximum spatial difference of 1000 km were selected as collocation criteria. We followed the respective data quality recommendations for each data set. To avoid comparisons of air masses inside and outside the polar vortex, we used sPV (scaled potential vorticity) from the GEOS-5 data assimilation system interpolated to the location and time of each of the observations. For $\delta^{17}O$, this approach is not applicable, as SMR does not measure $\rm H_2^{17}O$ and $\rm H_2^{16}O$ simultaneously. A climatological comparison was performed instead. In addition to these satellite intercomparisons, comparisons with other remote sensing data products are discussed.