Supplement of

The SPARC water vapour assessment II: profile-to-profile and climatological comparisons of stratospheric $\delta^2D(\text{H}_2\text{O})$ observations from satellite

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Preamble

This supplement consists of two parts. In the first part the sensitivity of the results on the \( \delta D \) derivation approach are discussed (Sect. 1). In the main part of this manuscript we distinguish between two approaches to derive a \( \delta D \) product (as an average for example) from a set of simultaneous HDO and H\(_2\)O observations, i.e. the “individual” and the “separate” approach. The latter approach is used consistently in the main part of the manuscript to allow comparisons on equal terms, given that the SMR observations do not provide simultaneous observations of HDO and H\(_2\)O. Here we use MIPAS and ACE-FTS data, which have simultaneous HDO and H\(_2\)O observations, to quantify the sensitivity of the \( \delta D \) results depending on the approach chosen. Section 1.1 focuses on the profile-to-profile comparisons, Sect. 1.2 on the comparisons of seasonally averaged latitude cross-sections and Sect. 1.3 on the comparisons of monthly averaged profiles in the tropics.

The second part provides a collection of figures (Sect. 2). As Fig. 1 in the main part of this manuscript comparisons of absolute \( \delta D \), HDO and H\(_2\)O profiles are shown, but here considering all (i.e. ten) data set combinations. This figure extends over multiple pages. The page headers provide a guidance on that and also indicate which data sets are compared to each other. Further, as Fig. 3 in the main part of this manuscript the \( \delta D \) climatologies for SMR, MIPAS and ACE-FTS are shown, but here for all seasons.
1 Sensitivity of the $\delta D$ derivation approach

1.1 Profile-to-profile comparisons

Figure S1 shows the bias estimates from the profile-to-profile comparisons of different MIPAS and ACE-FTS data sets using the “individual” approach. Compared to the results based on the “separate” approach, shown in Fig. 2 in the main part of the manuscript, both consistent and different features are observed. The most prominent differences are found towards the lower and upper altitude boundaries where the individual MIPAS and ACE-FTS data sets can be compared with each other. At the lower end the absolute biases exhibit a larger size for the “individual” approach than the “separate” approach. At the upper end the “separate” approach indicates negative absolute biases (or positive relative biases) while for the “individual” approach the results have often the opposite sign or are more close to zero. Also the comparisons among the two MIPAS and the two ACE-FTS data sets exhibit differences in details.

Figure S1: Profile-to-profile comparisons between different MIPAS and ACE-FTS $\delta D$ data sets based on the “individual” approach. As in Fig. 2 of the main manuscript, which shows the results of the “separate” approach, the x-axis has been reversed for the relative biases to achieve visual consistency with the absolute biases.
sensitivity of δD derivation approach

Figure S2: Differences between the “separate” and the “individual” approach for the seasonally averaged latitude cross sections at 100 hPa (left panels), 10 hPa (middle panels) and 1 hPa (right panels).
1.2 Comparisons of seasonally averaged latitude cross-sections

Figure S2 shows the differences between the two approaches (“separate” approach minus “individual” approach) for seasonally averaged latitude cross sections at 100 hPa (left panels), 10 hPa (middle panels) and 1 hPa (right panels). These results relate to Figs. 4 – 6 in the main part of the manuscript, which show the seasonally averaged latitude cross sections based on the “separate” approach for the three pressure levels considered here. Differences can be observed in all dimensions, i.e. season, altitude and latitude. The differences are typically within ±10 per mille with a few exceptions. At 100 hPa those are mostly located in the tropics and subtropics. The largest differences in absolute terms are however found in the Antarctic in JJA amounting to -25 per mille. At the higher altitudes the largest differences occur predominantly towards the polar regions. Overall, the differences are smallest at 10 hPa. At 1 hPa the differences are systematically negative, i.e. the “individual” approach results consistently in higher δD values than the “separate” approach at this altitude. At the other altitudes such systematic effect cannot be found and positive and negative differences are about equally distributed.

1.3 Comparisons of monthly averaged profiles in the tropics

Here we focus on the differences due to the two approaches with regard to the monthly averaged profiles in the tropics, relating to Fig. 10 in the main part of the manuscript. Figure S3 indicates similar vertical structures during all four months considered. Below 100 hPa very often positive differences can be observed, which occasionally exceed 50 per mille. Slightly above 100 hPa the MIPAS data sets indicate differences with the opposite sign. Those are larger than 10 per mille in absolute terms. Higher up the differences are small, typically amounting to a few per mille. Just at the upper altitude boundaries of the individual data sets again larger differences between the two approaches are visible.
sensitivity of δD derivation approach

Figure S3: As Fig. S2 but here focusing on monthly averaged profile in the tropics.

2 Figure collection

In the following a collection of figures as Fig. 1 and 3 in the main part of this manuscript are provided. In Fig. S4 comparisons of absolute δD, HDO and H2O profiles are shown for the 10 data set combinations. In Fig. S5 the δD climatologies are shown for the four seasons MAM, JJA, SON and DJF.
profile-to-profile comparison SMR v2.1 vs. MIPAS v20 (2 of 10)

Continued on next page
profile-to-profile comparison SMR v2.1 vs. ACE-FTS v2.2 (3 of 10)

Continued on next page
profile-to-profile comparison SMR v2.1 vs. ACE-FTS v3.5 (4 of 10)

Continued on next page
profile-to-profile comparison MIPAS v5 vs. MIPAS v20 (5 of 10)

Continued on next page
profile-to-profile comparison MIPAS v5 vs. ACE-FTS v2.2 (6 of 10)

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Envisat/MIPAS v5  SCISAT/ACE-FTS v3.5

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Figure S4: Profile-to-profile comparisons of the absolute δD, HDO, H2O profiles for the different data set combinations.
climatology MAM

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climatology JJA

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Figure S5: Climatologies of δD for the five data sets considered in this study and the four seasons MAM, JJA, SON and DJF (as indicated in the page headers).