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Supplement of

12 years of continuous atmospheric O_2, CO_2 and APO data from Weybourne Atmospheric Observatory in the United Kingdom

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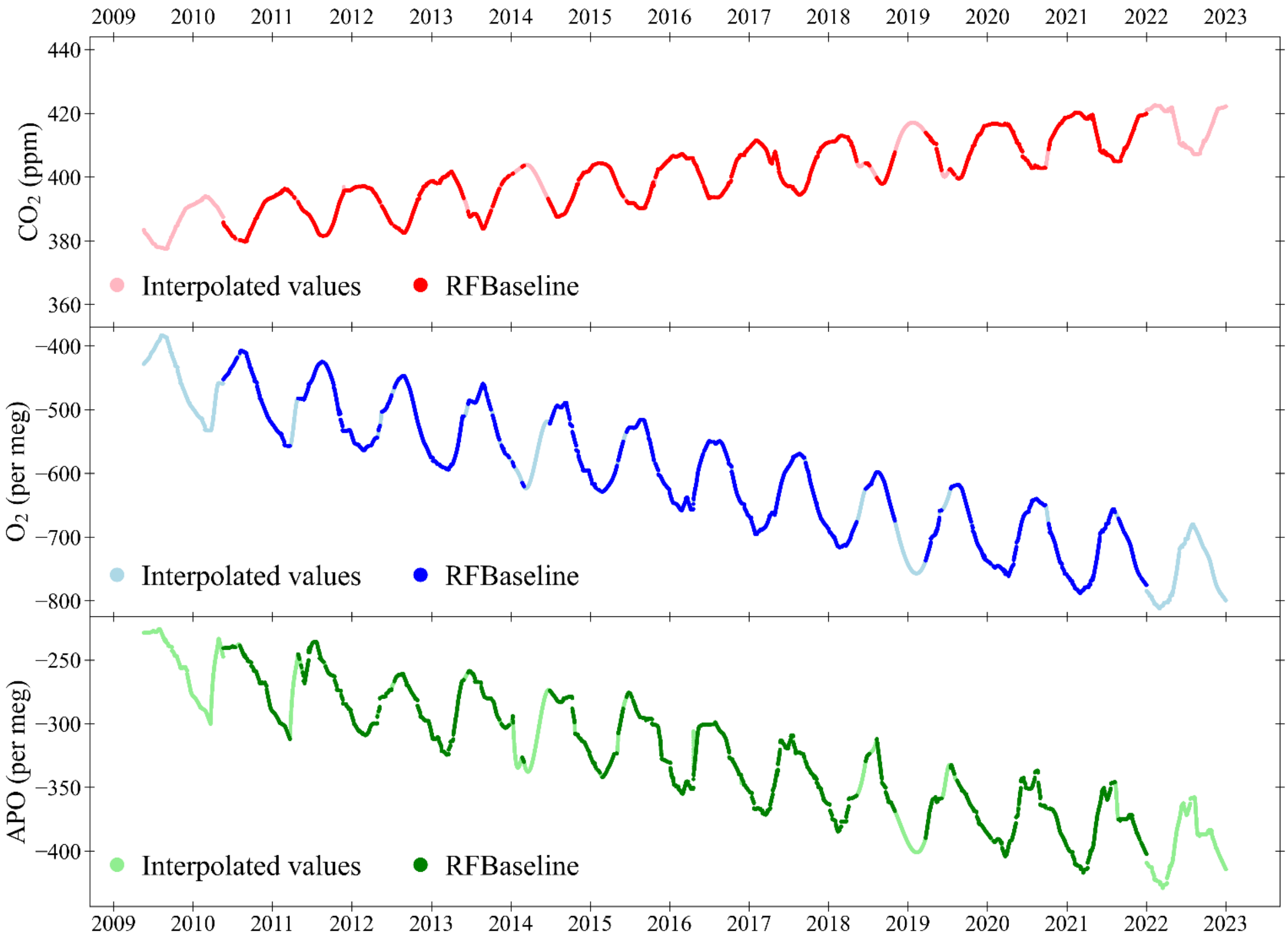

Figure S1: The CO_2, O_2 and APO time series baselines at WAO, calculated using the REBS method in the RFBaseline function within the IDPMisc package in R (Ruckstuhl et al., 2012; 2020). These baselines were interpolated to fill in the gaps where there are missing data using the na_seadec function in the imputeTS package. Missing data are either because of routine cylinder analyses, because of scheduled system maintenance, or because of inadvertent downtimes owing to system faults. The time series (2010-2021) were extended by a year both forwards and backwards in time (2009-2022) by taking the interpolated data for the first year and the last year and adding/subtracting the average annual long-term trends for each species. This was done to avoid possible end effects with the STL decomposition. The O_2 and CO_2 y-axes are scaled to be visually comparable on a mole per mole basis. The APO y-axis is zoomed in 2 times, compared to the O_2 y-axis on a mole per mole basis. The x-axis tick marks are at the beginning of each year.

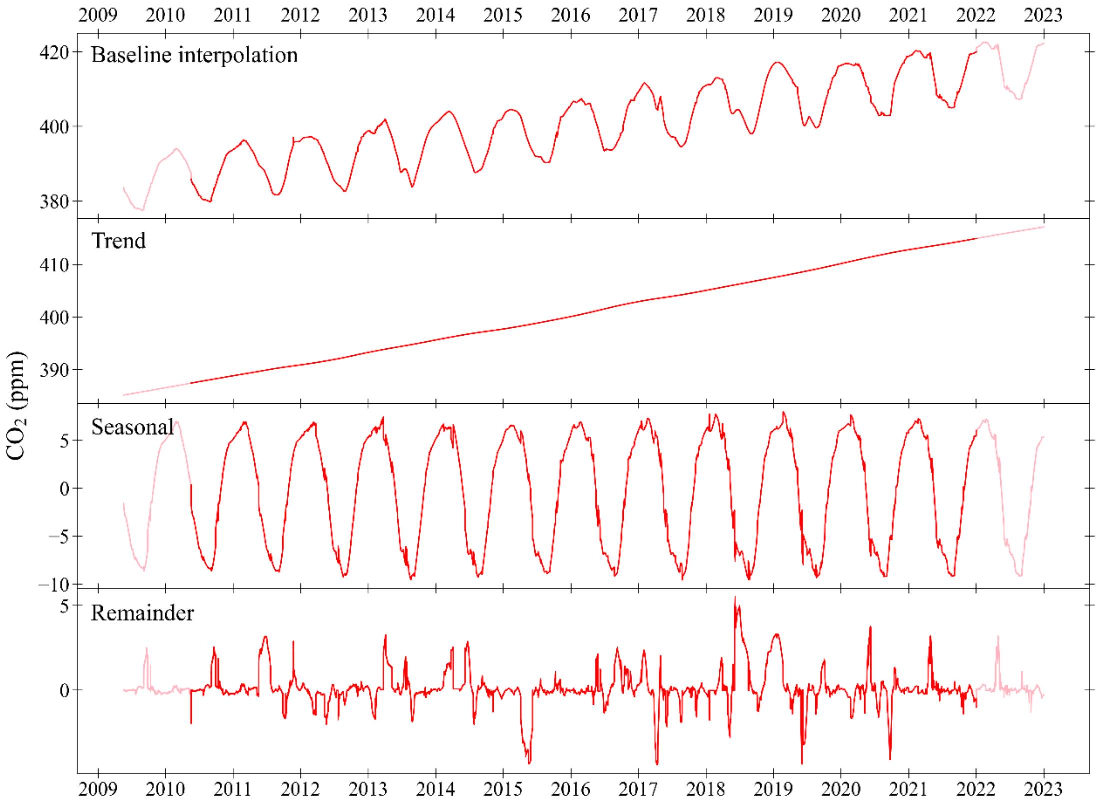

Figure S2: Time series decomposition of hourly averaged CO_2 amount fractions from WAO. The time series (2010-2021) was extended by a year both forwards and backwards in time (2009-2022) to minimize end effects. The top panel shows the data prior to decomposition, with the remainder, seasonal (detrended) and trend (deseasonalised) components plotted beneath respectively. 'Remainder' is calculated by subtracting both the seasonal and trend components from the baseline interpolated data. Vertical axis units are in ppm; the seasonal and remainder panels have been normalised to corresponding values of the long-term trend, which are denoted as 0 ppm. The decomposition was carried out using a curve fitting program called STL (see Sect. 2.3).

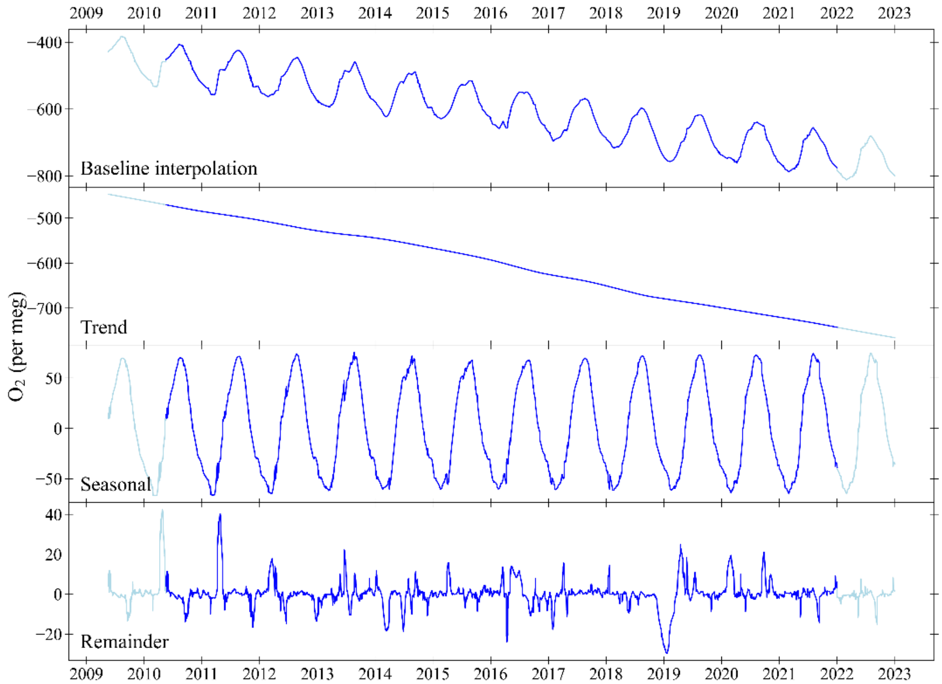

Figure S3: Same as for Fig. S2 but showing O_2 in per meg.

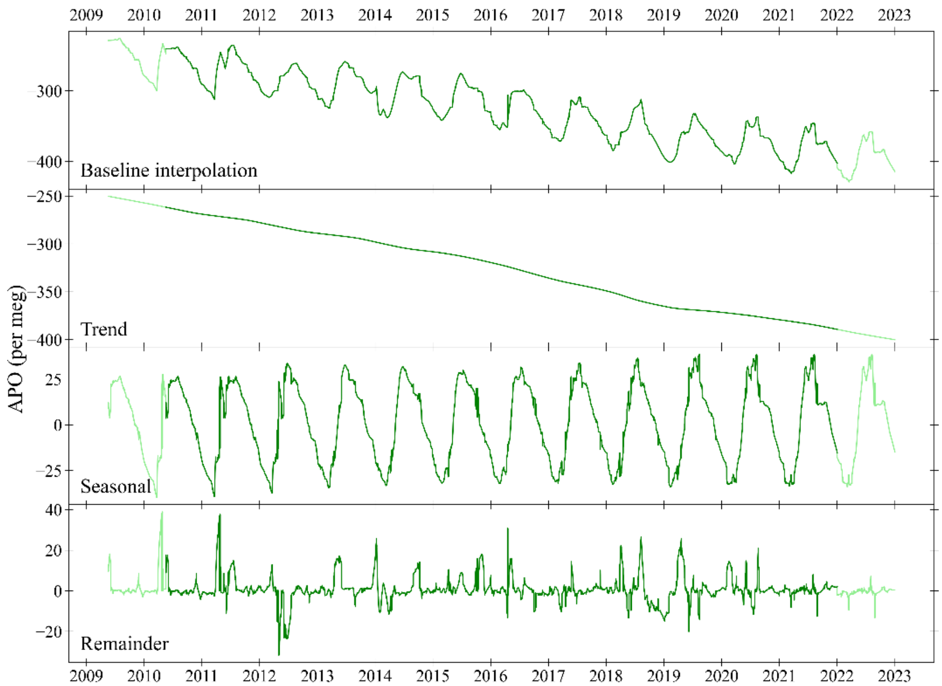

Figure S4: Same as for Fig. S2 but showing APO in per meg.

S1. Pump leak adjustment

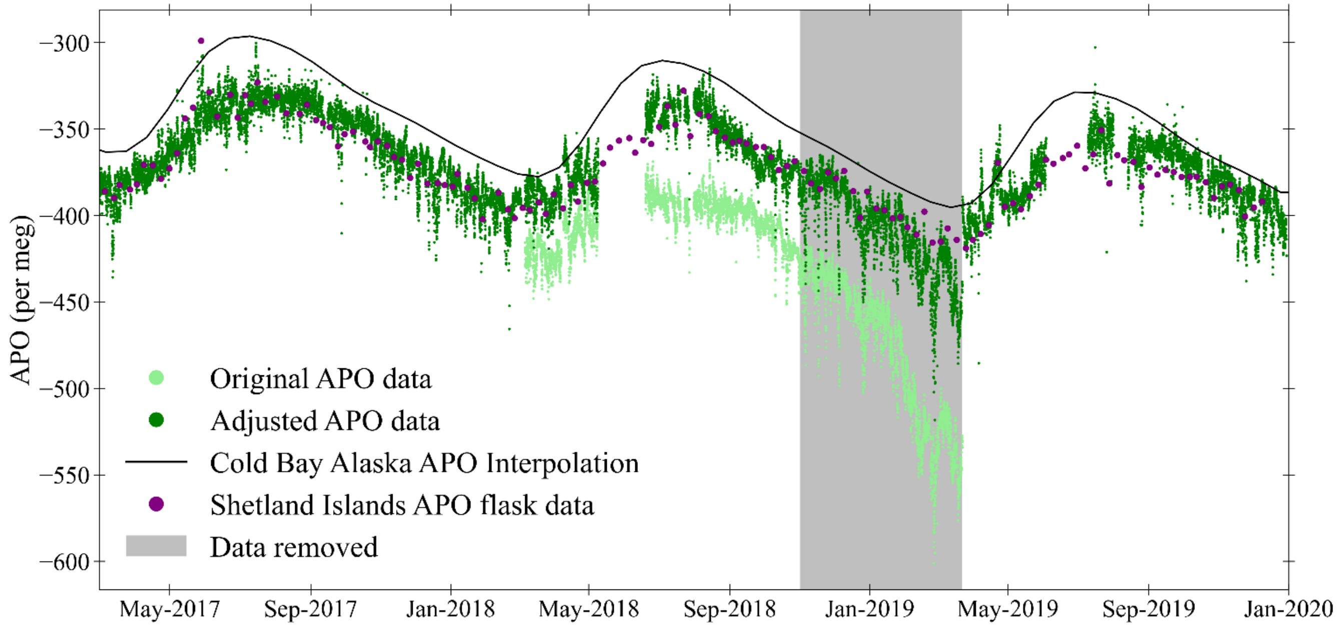

Figure S5. The original (light green) and adjusted (dark green) APO measurements at WAO from March 2017 to December 2019. Also, the Cold Bay Alaska APO data (black line) interpolated from flask samples and the Shetland Islands APO flask data (purple). The vertical grey bar shows the time period when the WAO data were removed.

From 6th March 2018 to 22nd March 2019 the diaphragm in one of the KNF pumps was torn causing the pump to leak. During this time only one of the inlet lines was being used so this leak affected all the O_2 data, as it caused the O_2 to fractionate (Keeling et al., 2007). The CO_2 data were not affected. There was a step change in O_2 between 2nd March 2018 and 6th March 2018 indicting that this is when the diaphragm originally tore, the data during this period has been excluded. The O_2 baseline then decreased over time indicating that the tear got gradually bigger. On 22nd March 2019 the diaphragm was replaced.

The leak changes all the data by a consistent amount over shorter timescales. To recover as much of these data as possible, we need to determine what the O_2 baseline would have been without the leak and then apply an adjustment to the data. The adjustment was done by comparing the WAO data to O_2 flask measurements from Cold Bay Alaska, U.S.A. (CBA, 55.2100° N, 162.72° W, https://scrippso2.ucsd.edu/data/cba.html). We determined a pre-leak period of 1st March 2017 00:00 to 2nd March 2018 22:00 and a leak period of 6th March 2018 15:00 to 22nd March 2019 10:00. The CBA O_2 measurements were interpolated to hourly values. We used the RFBaseline function in R, on the WAO hourly data for the pre-leak period and the leak period (span: 0.114 preleak, 0.110 leak, maxit: (3,0), b: 0.0001). The WAO baseline was then interpolated from hourly data to 2-minute data. We then took the difference between the WAO baseline and the CBA interpolation for each month during the pre-leak period and adjusted the WAO baseline for the leak period, so the difference was the same as the pre-leak period e.g., the average difference in July 2017 (pre-leak) is used to adjust the O_2 data in July 2018 (during leak). The adjusted WAO O_2 data were then used to recalculate APO. Figure S5 shows the APO data during the leak-period, as it is easier to see the changes with APO than with O_2.

The APO data were compared to APO data from Shetlands Island, Scotland (SIS, 60.28°N, 1.28°W, https://doi.org/10.17617/3.ZQX1LI). Even after the adjustment there was still a step change in APO between the end of the leak period and the beginning of the post-leak period. Also, there were lots of large downward spikes towards the end of the leak period. It was determined that the leak was so big by this point that it could not be adjusted for. Therefore, the O_2 data from 1st November 2018 00:00 to 22nd March 2019 10:00 has been excluded.