Supplement of

New sampling strategy mitigates a solar-geometry-induced bias in sub-kilometre vapour scaling statistics derived from imaging spectroscopy

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Real-world water vapour ($q$) fields have complicated 3-D structures. The main manuscript uses large-eddy-simulation outputs to represent these 3-D structures but this supplement uses simplified fields to illustrate how directional solar geometry affects derived scaling statistics. For this purpose, assume a uniform $q$ field above 1 km deep PBL, within which the field varies with some structure in the $x$ direction. Each 50 m column within the PBL has an assigned total $q$, but within each column the PBL $q(z)$ profile is uniform.

The downward path-integrated vapour along the solar direct beam for SZA=45° and solar azimuth of 90° ($x$ direction) or 0° ($y$ direction) is compared with the raw field in Figure S1. The raw field is visibly smeared in the solar azimuth direction (panels b—c). The field mean at each $x$ (i.e. averaging values along $y$ for each $x$ location) are displayed in panels d—f. From (e), calculating the field statistic along the same direction as the smoothing (i.e. “parallel” to the smoothing) introduces a spatially-varying mean bias, which is eradicated when calculating in the $y$ direction (i.e. “perpendicular”). This spatially-varying mean bias will introduce additional variance to $S_2$ as a function of separation $r$, when calculating in the $x$ direction.

This principle is conceptually similar to motion blur in images, in that long-exposure images are smoothed in one direction, and characteristic structures of the static image are maintained depending on their orientation with regards to the motion. However, we use the term “smearing” rather than “blurring” to distinguish our results from those related to physical movement.

In Figure S2 it can be seen that smoothing reduces the absolute value of $S_2$ regardless of direction, this is a consequence of averaging over the random noise in Figure S1(a). Panel (b) shows how, when calculated parallel to the solar azimuth, $S_2$ varies greatly with separation distance, compared to the true field $S_2$. This separation-dependent variation will change the derived $\zeta_2$. Meanwhile the perpendicular calculation greatly mitigates this separation-dependent bias.

Finally, Figure S3 reports the bias in $\zeta_2$ calculated for separations of 0.5—1 km as a function of SZA. There is a substantial bias in the parallel calculation that is mitigated by performing only a perpendicular calculation. The bias is effectively eliminated for low SZA, but by SZA=60° the perpendicular bias rises to about 10 % of that of the parallel calculation, i.e. for this field and geometry, our sampling strategy reduces the bias by 90 %.

These calculations were only applied for the downward path-integrated water vapour through a highly idealised and unrealistic field. However, it is intended only to illustrate how solar azimuth affects path-integrated vapour, and therefore changes the structure of 2-D fields of VSWIR-retrieved TCWV. These results show clearly that our method of calculating perpendicular to the solar azimuth can mitigate these biases, and the main manuscript performs this analysis on realistic 3-D $q$ fields while accounting also for the upward solar path to a nadir-viewing sensor.
Figure S1 (a) Randomly generated 2d field, (b) field smoothed in the x direction, (c) field smoothed in the y direction. The smoothing represents the effect of SZA>0° where columns are vertically uniform with a solar azimuth in either the x or y direction. (d) mean along y direction of field in raw field, (e) mean after x smoothing, and difference relative to the raw mean, (f) mean after y smoothing, and difference relative to the raw mean.

Figure S2 (a) Second-order structure functions calculated as a function of separation distance from each of the fields in Figure S1, (b) the differences between $S_2$ from the smoothed fields relative to the true value from the raw field. The blue line (“parallel”) represents calculation along x and the orange line (“perpendicular”) represents calculation along y.
Figure S3. Bias in calculated exponent over 500—1000 m separation for the fields in Figure S1 presented as smoothed minus truth. Calculating perpendicular to the solar azimuth (orange) reduces in far smaller biases than perpendicular (blue).