



Supplement of

Application of the Complete Data Fusion algorithm to the ozone profiles measured by geostationary and low-Earth-orbit satellites: a feasibility study

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Fusion of 1000 pixels in coincidence

Here, the CDF is applied to 1000 coincident L2 measurements that refer to the same true profile, the same AK matrix and the same CM but have different (noise) errors δ_i randomly generated according to Eq. (3). The 1000 products have been simulated according to the specification of GEO platform and thermal infrared (TIR) band. It is noted that the particular type of product is of secondary importance in this example, which aims to evaluate the behaviour of the fusion of many coincident measurements of the same type that only differ by the random error. In the left panel of Figure S1 the profile obtained fusing 1000 coincident L2 products is compared with their arithmetic average, with the true profile and with the a priori profile. Since in this case the 1000 pixels are coincident in space and time, no coincidence error $\delta_{coinc,i}$ was added in the CDF formulas of Eqs.(6).

In the right panel of Figure S1, the deviations of the fused profile (hereafter indicated with FUS), of the average value of the L2 measurements (indicated as <L2>) and of the a priori profile from the true profile are shown. In the same panel, the estimate of the total error standard deviation σ_{total} that characterize each of the 1000 L2 profiles (calculated as the root square of \mathbf{S}_{total} , Eq. (5)), the estimate of the total error standard deviation of FUS profile σ_{ftotal} (calculated as the root square of \mathbf{S}_{total} , Eq. (5)) and the estimate of the total error standard deviation of the average of the L2 measurements (calculated by dividing σ_{total} by $\sqrt{1000}$, as if no bias is present) are also represented. It is worth noticing that $\sigma_{total}/\sqrt{1000}$ is much smaller than the observed (<L2> minus true) differences, suggesting the presence of a bias. A clear similarity of these differences with the shape of the (a-priori minus true) profile can be observed indicating a link between this bias and the a priori information. The fused profile provides instead a better representation of the true profile with residuals that are consistent with the estimated errors, although these are much larger than $\sigma_{total}/\sqrt{1000}$.



Figure S1 Left panel: Vertical Ozone Volume Mixing Ratio (VMR) profiles. The blue line represents the true profile; the black line indicates the a priori used in the L2 simulations (the same for all the 1000 L2 products) that is also the one used to constrain the fused profile, represented in dark red. The green line represents the average of the 1000 simulated profiles and the grey shaded area centred on the green line represents the standard deviation of the L2 total error (the same for all the 1000 L2 products). **Right panel:** the green and the dark-red lines represent respectively the difference between the <L2> average and the FUS profile from the true profile. The magenta dash-dotted profile represents the difference between the a priori and the true profiles. The dotted black line represents the standard deviation of the 1000 L2 measurements. The dash-dotted dark-red line represents the standard of the FUS product. The dotted green line is the standard deviation of L2 total error estimate of the FUS product. The dotted green line is the standard deviation of L2 total error estimate divided by $\sqrt{1000}$

Recalling Eq. (8), it is the term $(I - A)(x_a - x_t)$ that causes the bias observed in the right panel of Figure S1. Figure S2 compares the amplitude of the bias term $(I - A)(x_a - x_t)$ with the mean total error. For illustration, the total errors

computed when only considering either 5 or 10 individual measurements are also plotted. As it can be noticed, the mean total error tends to the bias term as the number of profiles increases. When a large number of profiles are considered (order of 1000) the mean total error substantially coincides with the bias itself.



Single grid-box analysis (1°x1°)

A single 1°x1° cell is considered (Figure S3) that contains the 0.5°x0.625° cell represented in Figure 1, where in this new example 361 L2 measurements are fused together (168 GEO-TIR, 168 GEO-UV1, 23 LEO-TIR, 2 LEO-UV1).



Comparing Figure S4 with the correspondent left panel of Figure 2 in the paper, that refers to the 0.5°x0.625° cell, it can be observed that while the *FUS total error* decreases augmenting the number of fused measurements, the *FUS*-

*<true>*differences show a little increase in their maximum value but still remain much lower than individual *L2-true* differences.



It is also interesting to look at the diagonals of the AK matrices of Figure S7 and to compare them with the ones of the left panel of Figure 3 obtained with 118 fused measurements. The FUS average number of DOFs increase from 9.59 (Figure 3) to 12.16 if all the 361 L2 measurements are considered (Figure S5, DOFs FUS). The number of DOFs are 10.85 when only 359 measurements are fused, disregarding the two LEO UV ones (Figure S5, DOFs FUS(*)). In other words, if the number of L2 measurements passes from 118 to 359 the average number of DOFs increases by 1.26. On the other hand, the addition of two more measurements with information content significantly higher than all the others increases the average number of DOFs of 1.31. In particular in Figure S5 is evident that the contribute of the LEO UV measurements to the fusion is significant at higher altitudes, where their information content is sensibly higher than in the other kinds of L2 products.



Statistical analysis for a large domain (cell size 1°x1°)

Figure S6 shows the *SF DOF* obtained in the case of a $1^{\circ}x1^{\circ}$ resolution (Table 4). A test of the flexibility of the data fusion procedure is the objective of this analysis and, for simplicity, the same coincidence error used for the higher resolution grid (0.5°x0.625°) was adopted. The adaptive choice of the amount of coincidence error to be used in the fusion is currently an open issue in the CDF development and is discussed in Ceccherini et al. (2019). In Figure S6 the *SF DOF* increases linearly with the logarithm of the number of L2 fusing profiles, like in Figure 6, and with a similar rate of growth so that Figure S6 looks like an extrapolation of Figure 6, for greater values of *N*. This is because the same types of L2 measurements as in the previous case are being fused.

Figure S7 shows the *SF AK* and *SF ERR* now computed for the coarse resolution grid and for the 775 FUS products considered in Table 4. The greater number of fusing observations with respect to Figure 7 produces a general improvement for both the AK diagonal values and the total error, although in the figures it is difficult to detect the first improvement because of the logarithmic scale. The CDF method can be used with a wide range of grid-box size and data compression and the quality of the products generally improves with larger cells. An upper limit to the grid-box size is caused by the requirement of a coincidence error amount, which degrades the quality of the fused product.

Figure S7. *Left panel: SF AK* versus vertical level. *Right panel: SF ERR* versus vertical level. In both panels, different colours of the symbols represent the FUS type, different sizes of the symbols represent the number of products that have been fused. The maximum symbol size shown in the legend corresponds to N=504.