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Supplement of

An assessment of the climatological representativeness of IAGOS-CARIBIC trace gas measurements using EMAC model simulations

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S1 Introduction

This supplement discusses further results of the study of the representativeness of IAGOS-CARIBIC data using the chemistry-climate model EMAC. For abbreviations and methods, please refer to the main text. Two points are discussed here:

The methods to describe representativeness developed and tested with model data were also applied to data from a random number generator. This is described in Section S2. Section S3 discusses the sensitivity study of the Kolmogorov-Smirnov test using a subsample of $\text{MOD}_{\text{CARIBIC}}^{\text{regular}}$.

S2 Calculating representativeness from random numbers

All three methods to investigate representativeness (Kolmogorov-Smirnov test, variability analysis and relative differences) have also been applied to data created with a random number generator. The results of this study are presented here.

To produce the random numbers, 20 sets of 10^8 numbers were taken from a normal distribution. These 20 sets are referred to as species, well aware of the fact that they are purely artificial. From species to species, the standard deviation σ was set to vary from 10^{-3} to 10^3, values of the exponent increasing linearly. 20 mean values μ (increasing from 10^4 to 10^8, with a linear increase in the exponent) where distributed randomly to the 20 species. This results in 20 species with different values for σ and μ. The statistics of each species will be indexed by the number 2. For short, this dataset will be called RAND.

3000 samples were taken from each of the 20 species. For each sample, 20 numbers were first randomly drawn from each species. These new numbers and all those that had been drawn before then make up this one sample. So the size increases by 20 for each sample. This way, the relationship of the representativeness score with the sample size is directly accessible. Samples are indexed by the number 1.

The variability τ^* of each species is defined as in Equation 3 of the main text: $\tau^* = \log_{10}(\sigma_2/\mu_2)$. The two requirements set up in Section 3.3 for representativeness in general also have to hold here:

1. Representativeness has to increase with the number of samples.

2. Representativeness has to decrease with increasing variability of the underlying distribution.

With RAND defined in this way, it is possible to test representativeness using the variability analysis following Rohrer and Berresheim (2006) and Kunz et al. (2008) (see Section 4.2) and the relative differences (see Section 4.3). The Kolmogorov-Smirnov test was positive for very few samples (less than fifty numbers, independent of τ^*) and will not be
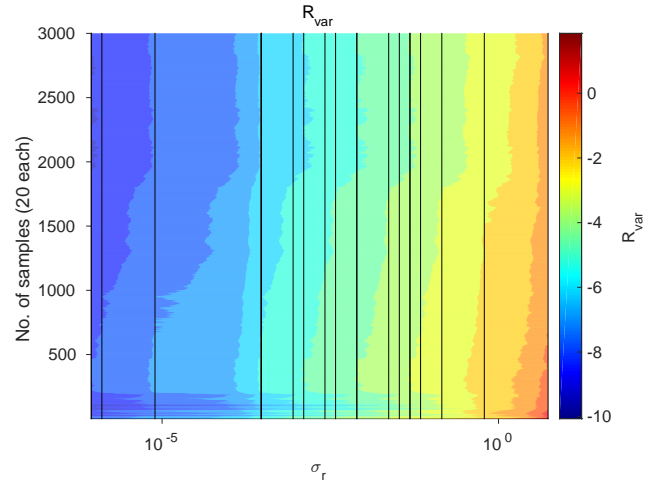

Figure S1. Representativeness score R_{var} applied to RAND. Vertical lines indicate the values of τ^* of each species.

further discussed. Its behaviour with aircraft data was subject of a sensitivity study, the results of which are shown in Sec. S3 of this supplement.

S2.1 Variability analysis

The variability analysis (defined in Section 4.2 and Eq. 3) was applied in a simplified manner. As RAND is independent of time, R_{var} is reduced to just a single value containing the absolute difference of variability of each species of RAND and the sample taken thereof: $\text{R}_{\text{var}} = |\nu_1 - \nu_2|$, where ν is the mean variability. Figure S1 shows a result. The exact result is a matter of chance, as a random number generator is used. Similar to using $\text{MOD}_{\text{CARIBIC}}^{\text{regular}}$ and $\text{MOD}_{\text{RANDPATH}}$, a strong dependance on τ^* and a weak dependance on the number of samples is visible.

Similar to R_{var} when using $\text{MOD}_{\text{CARIBIC}}^{\text{regular}}$ and $\text{MOD}_{\text{RANDPATH}}$, the variability analysis using RAND meets the two requirements necessary for describing representativeness, which were described in Section 3.3 and above. This result supports the finding that R_{var} can be used as a statistic for describing representativeness.

S2.2 Relative differences

Similar to R_{var}, R_{rel} is reduced to a simple relative difference when using RAND: $\text{R}_{\text{rel}} = |\mu_1 - \mu_2|/\mu_2$, where μ is the mean of the sample (index 1) and of the whole subset (index 2). Figure S2 shows a result when applying R_{rel} to RAND. The dependance on τ^* is strong and linear. The result also depends on the number of samples, showing a slow increase with the number of samples. This dependance is sometimes disturbed by better values which are reached by chance when drawing from RAND.
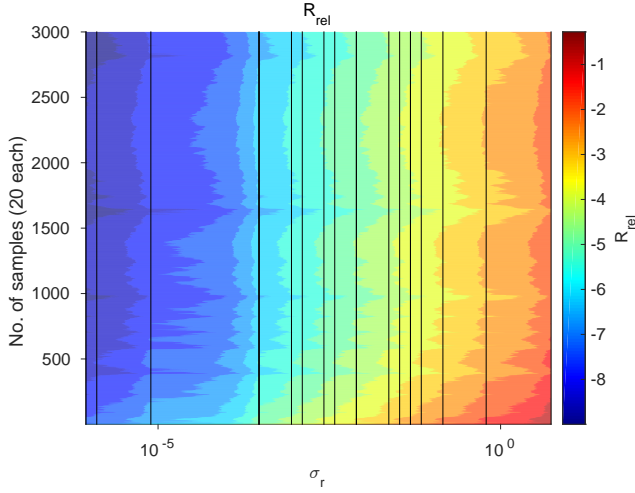
Figure S2. Like Figure S1, but for R_{rel}.

Like for $MOD_{CARIBIC}^{regular}$ and $MOD_{RANDPATH}$, R_{rel} passes both conditions for a valid description of representativeness: it depends on variability τ^* and on the number of samples. The latter is also being influenced by chance and generally much weaker.

The fact that R_{rel} passes the two conditions for a description of representativeness can be understood with some theoretical considerations. The standard error of the mean is defined by

$$\sigma_{\overline{x}} = \frac{\sigma}{\sqrt{n}} \tag{S1}$$

where $\sigma_{\overline{x}}$, the standard deviation of a sample, can be given by the following equation (N being the number of samples):

$$\sigma_{\overline{x}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\overline{x}_i - \mu)^2} \tag{S2}$$

For $N = 1$, this gives:

$$\sigma_{\overline{x}} = |\overline{x}_i - \mu| \tag{S3}$$

Plugging Eq. S3 into Eq. S1 gives:

$$\frac{|\overline{x}_i - \mu|}{\mu} = \frac{\sigma}{\mu\sqrt{n}} = \frac{10^{1/\tau^*}}{\sqrt{n}} \tag{S4}$$

and therefore

$$R_{rel} = \log_{10}\left(\frac{|\overline{x}-\mu|}{\mu}\right) = -0.5\log_{10}(n) + \frac{1}{\tau^*} \tag{S5}$$

So ideally, R_{rel} should depend inversely on τ^* and directly on the logarithm of the number of values. Figure S2 shows this is approximately true for RAND.

In the case of RAND, R_{rel} and R_{var} can both be used to describe representativeness as they pass the two conditions. Theoretical considerations make the finding plausible for R_{rel}. RAND can be considered a theoretical abstraction of MOD. The finding here therefore strongly supports that of Sections 5.2 and 5.3, where R_{rel} and R_{var} have also been found to be good descriptors of representativeness when using $MOD_{CARIBIC}^{regular}$ and $MOD_{RANDPATH}$ or $MOD_{RANDLOC}$. In the main text, we use R_{rel} for final results, as it more suitable to answer the question of representativeness for a climatology.

S3   Sensitivity study on the Kolmogorov-Smirnov test

When applying the Kolmogorov-Smirnov test to $MOD_{CARIBIC}^{regular}$, $MOD_{RANDPATH}$ or $MOD_{RANDLOC}$, it returned almost only negative results. This indicates that $MOD_{CARIBIC}^{regular}$ is not representative of $MOD_{RANDPATH}$ in the definition of the Kolmogorov-Smirnov test. This behaviour was tested in a sensitivity study, the results of which are discussed here.

One of the most frequent destinations within the CARIBIC project is Vancouver, Canada (near $120\,°W$, $45\,°N$, see Figure S3), and only the subset of $MOD_{CARIBIC}^{regular}$ to this destination is considered in this example to minimize effects that may come from different flight routes. Parts of this reduced dataset were tested with the Kolmogorov-Smirnov test against the whole reduced dataset for all variables. To produce these partial datasets, each flight was cut into an increasing number of pieces (corresponding to a certain time) and different percentages of these pieces were used in testing. Figure S3 shows an example of applying this method, by cutting each flight into 20 pieces and taking 30% of these by showing the corresponding flightpaths.

Data was not binned in months. When applying the Kolmogorov-Smirnov test without binning in months, the result is a profile in HrelTP for each variable. The result can then be diplayed in similar way to Figures 7 and 8. This matrix of height versus species was calculated for each combination of number of pieces and percent of pieces. In each combination, all the profiles of the different variables were averaged to end up with one value betwween 1 and 0 characterizing the result of the test for this combination of number of pieces and percent of pieces. The result can then give an impression of the strictness of the Kolmogorov-Smirnov test.

Figure S4 shows the result of the study. Independent of the number of pieces, the result is positive if all pieces are considered, as the definition of the test prescribes. But only when removing short pieces (shorter than $20\,min$) is the result also positive for less pieces, even though 70% percent of the data is still needed. When removing whole flights (at the top of the plot), more the 90% of the data has to be taken into account to achieve a positive result of the Kolmogorov-Smirnov test. This result is very similar also for other error
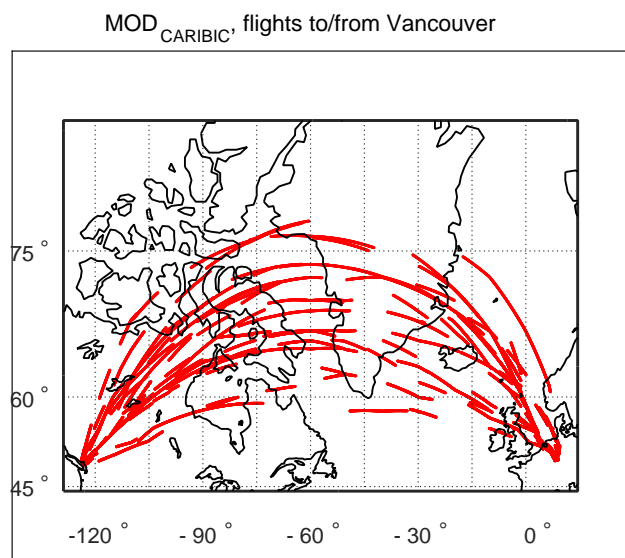
MOD$_{\text{CARIBIC}}$, flights to/from Vancouver

Figure S3. Flightroutes to Vancoucer, Canada, where each flight has been cut into 20 pieces and randomly chosen 30% of those pieces have been plotted. These are tested against the whole data from flights to Vancouver to give one point in Figure S4.

probabilities α, taking values of 0.001, 0.01, 0.05 (in the figure), 0.1 and 0.2. The area of failing increases only slightly with the error probability. This showcases the strictness of the test. The Kolmogorov-Smirnov test does not seem suitable to test a dataset measured with aircraft for representativeness of a larger dataset.

References

Kunz, A., Schiller, C., Rohrer, F., Smit, H., Nedelec, P., and Spelten, N.: Statistical analysis of water vapour and ozone in the UT/LS observed during SPURT and MOZAIC, Atmospheric Chemistry and Physics, 8, 6603–6615, 2008.

Rohrer, F. and Berresheim, H.: Strong correlation between levels of tropospheric hydroxyl radicals and solar ultraviolet radiation, Nature, 442, 184–187, 2006.
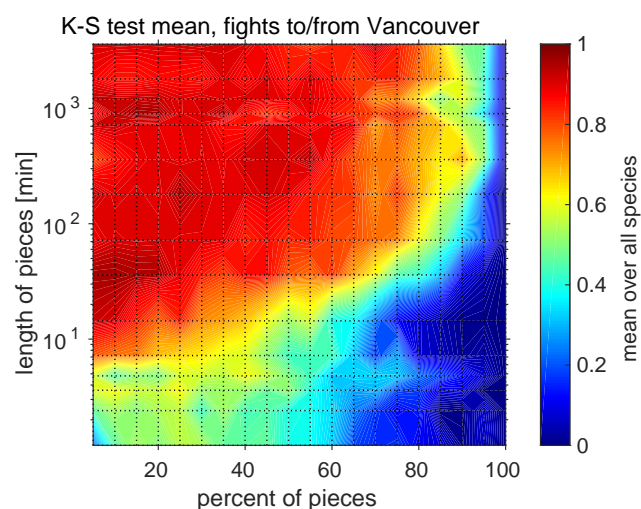
K-S test mean, fights to/from Vancouver

Figure S4. The Kolmogorov-Smirnov test applied to the flights to Vancouver, Canada, of MOD$_{\text{CARIBIC}}^{\text{regular}}$ and subsets of these flights. Dotted lines indicate those lengths in time and those percentages that were tested. 0 stands for a passing the Kolmogorov-Smirnov test, 1 for not passing.