atmosphere

Supplementary Materials: Share of Discontinuities in the Ozone Concentration Data from Three Reanalyses

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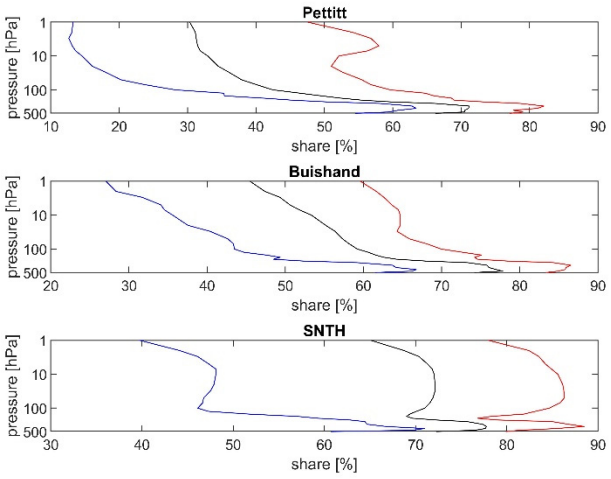


Figure S1. Vertical profile of average (black), minimal (blue) and maximal (red) share of discontinuities to all grids from all months from ERA-5 for the Pettitt test (upper panel), the Buishand test (middle panel), and the Standard Normal Homo-geneity test (SNTH, lower panel).

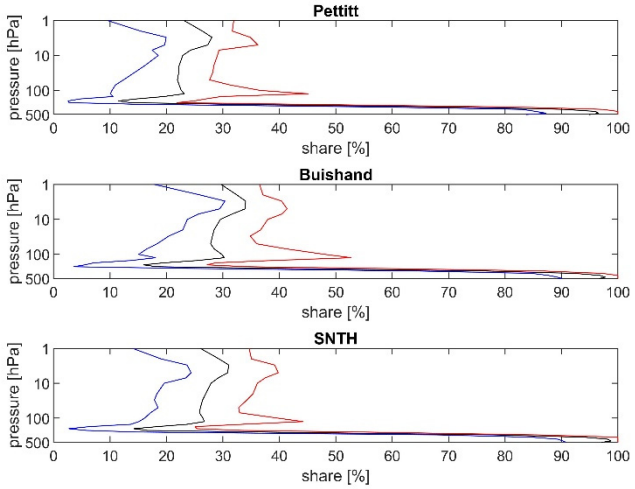


Figure S2. The same as Figure S1, but for JRA-55.

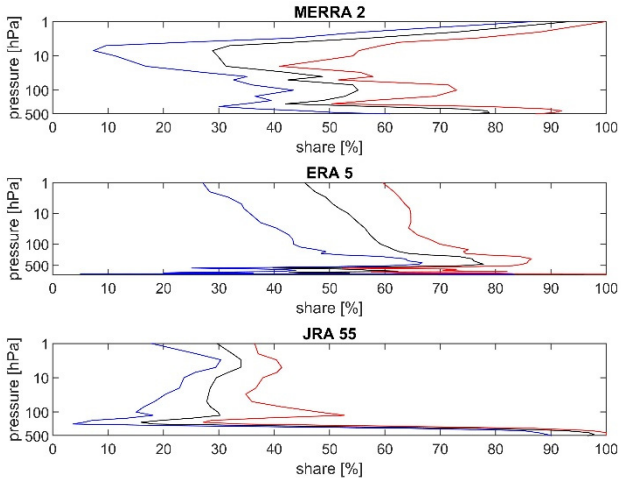


Figure S3. Vertical profile of average (black), minimal (blue) and maximal (red) share of discontinuities to all grids from all months from the Buishand test for MERRA-2 (upper panel), ERA-5 (middle panel), and JRA-55 (lower panel).

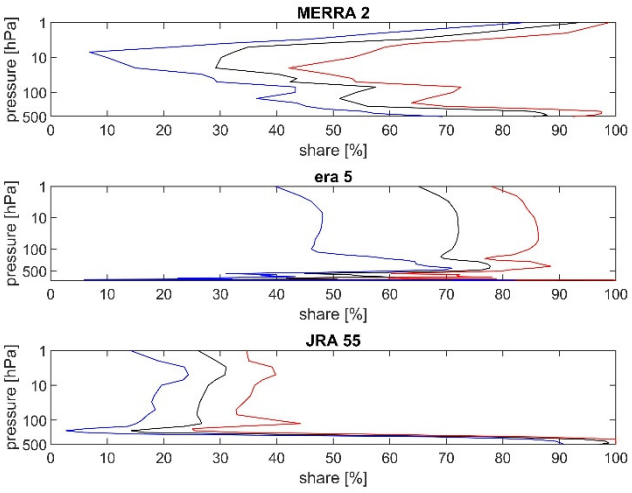


Figure S4. The same as Figure S3, but for the Standard homogeneity test.

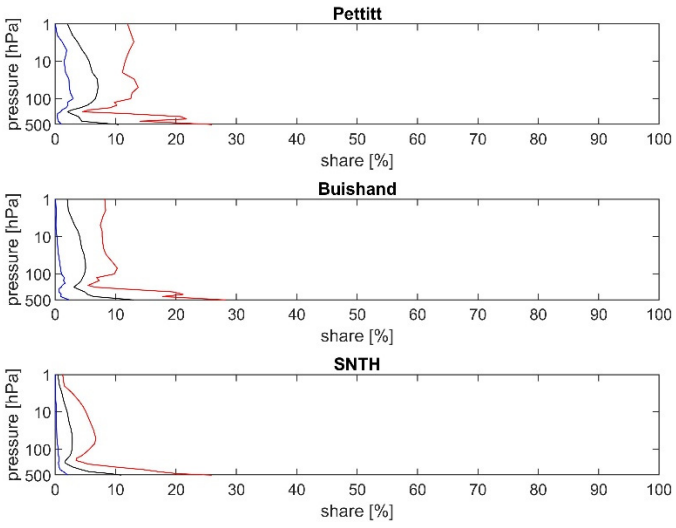


Figure S5. Vertical profile of average (black), minimal (blue) and maximal (red) share of explained discontinuities by the change in 2004 to all discontinuities from all months from ERA-5 for the Pettitt test (upper panel), the Buishand test (middle panel), and the Standard Normal Homogeneity test (lower panel).

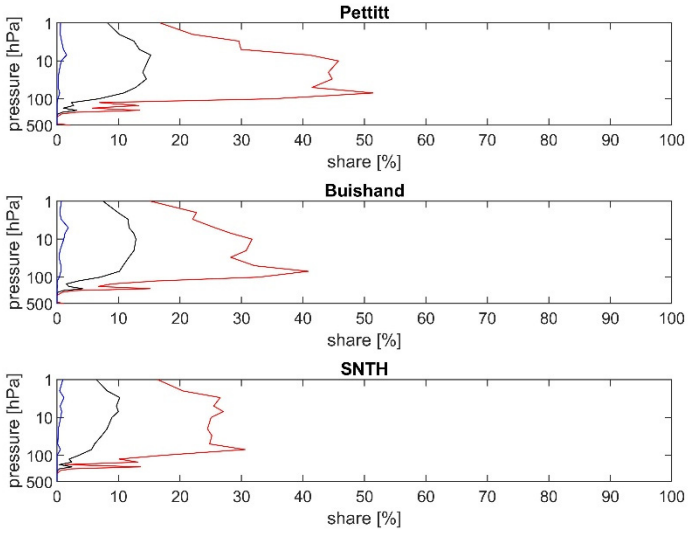


Figure S6 The same as Figure S5, but for JRA-55.

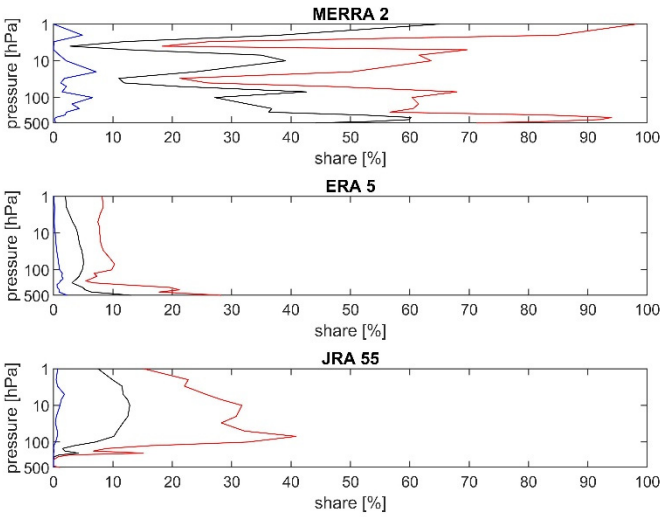


Figure S7. Vertical profile of average (black), minimal (blue) and maximal (red) share of explained discontinuities by the change in 2004 to all grids from all months from the Buishand test for MERRA-2 (upper panel), ERA-5 (middle panel), and JRA-55 (lower panel).

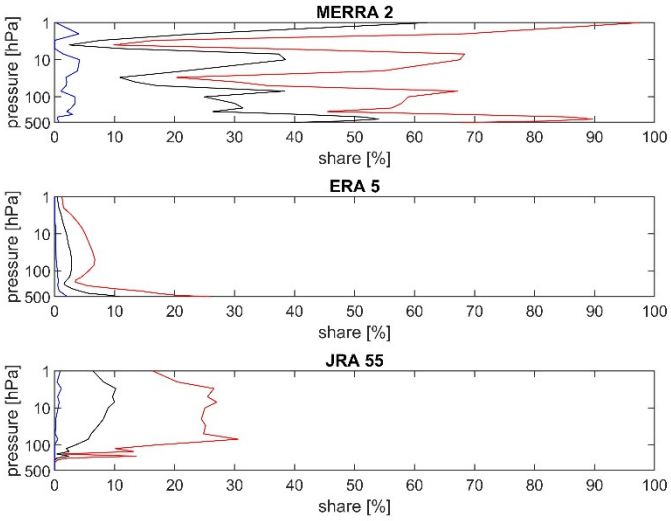


Figure S8. The same as Figure S7, but for the Standard homogeneity test.

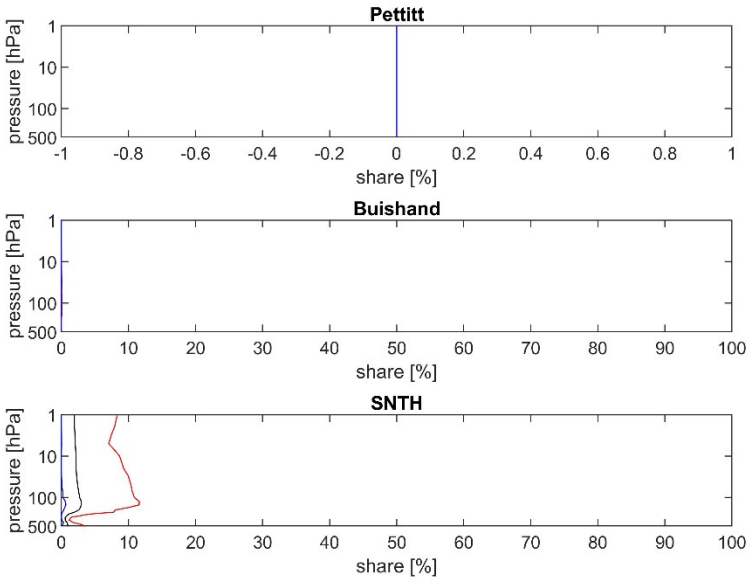


Figure S9. Vertical profile of average (black), minimal (blue) and maximal (red) share of explained discontinuities by the change in 2015 to all discontinuities from all months from ERA-5 for the Pettitt test (upper panel), the Buishand test (middle panel), and the Standard Normal Homogeneity test (SNTH, lower panel).

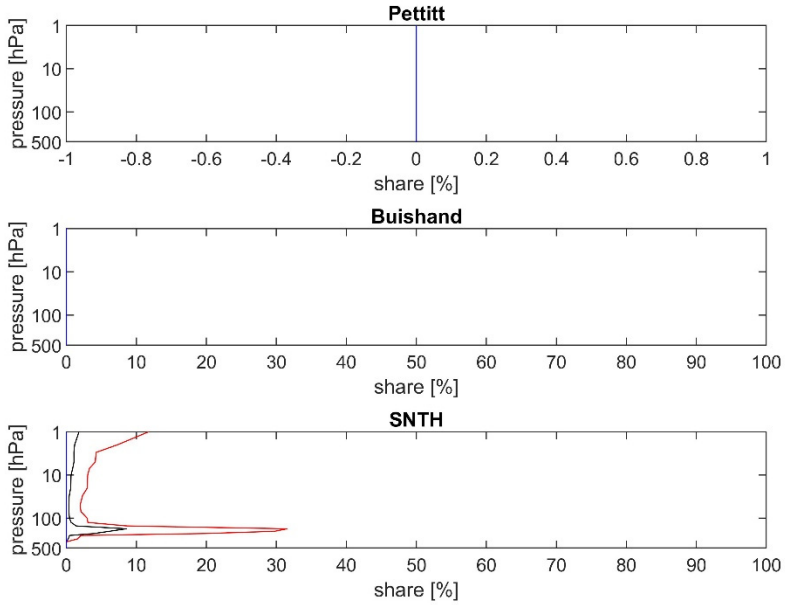


Figure S10. The same as Figure S9, but for JRA-55.

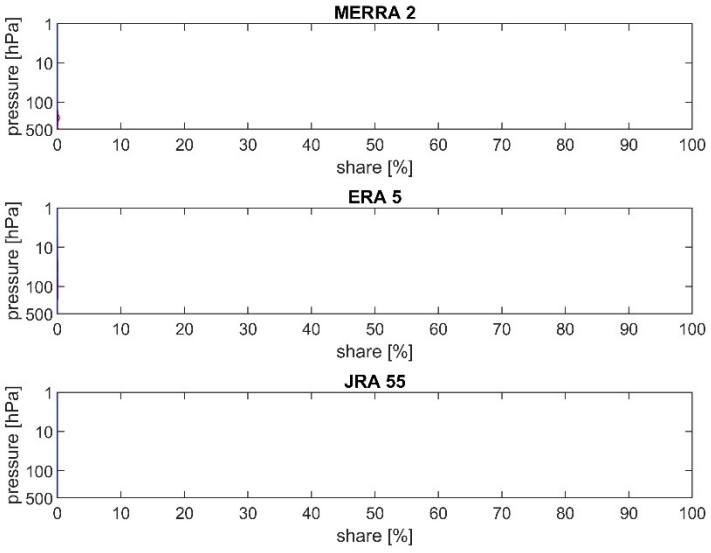


Figure S11. Vertical profile of average (black), minimal (blue) and maximal (red) share of explained discontinuities by the change in 2015 to all grids from all months from the Buishand test for MERRA-2 (upper panel), ERA-5 (middle panel), and JRA-55 (lower panel).

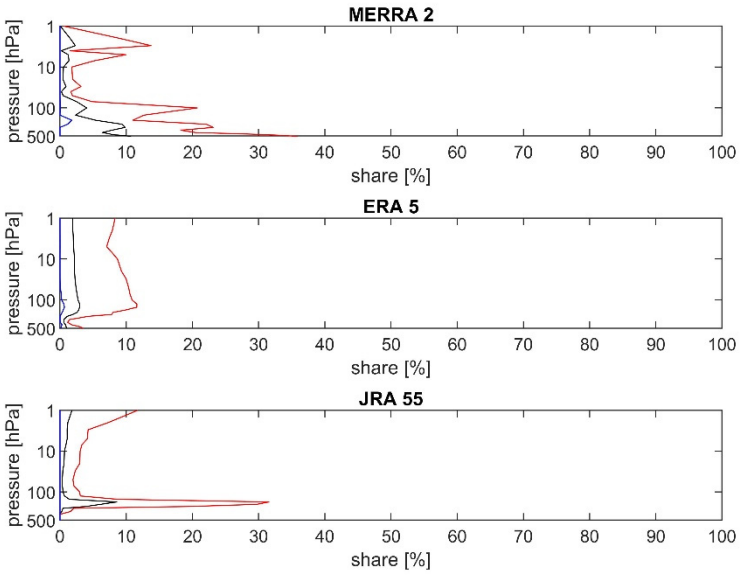


Figure S12. The same as Figure S11, but for the Standard homogeneity test.

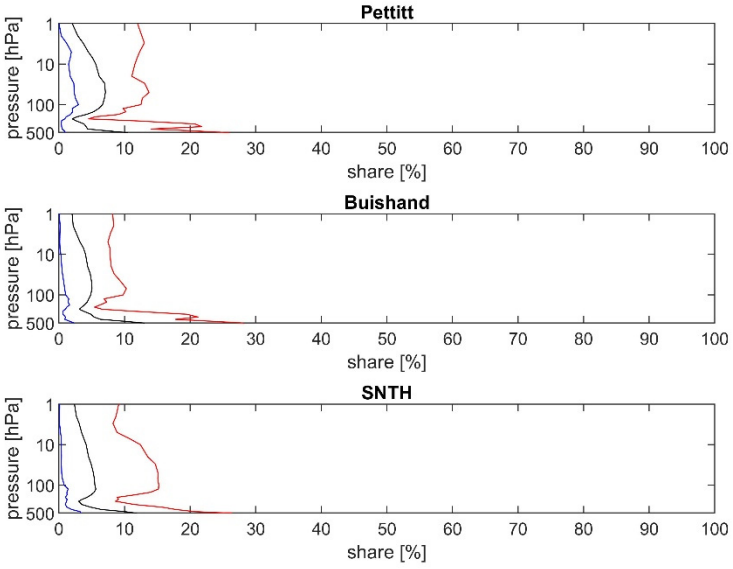


Figure S13. Vertical profile of average (black), minimal (blue) and maximal (red) share of explained discontinuities by the change in 2004 and in 2015 to all discontinuities from all months from ERA-5 for the Pettitt test (upper panel), the Buishand test (middle panel), and the Standard Normal Homogeneity test (SNTH, lower panel).

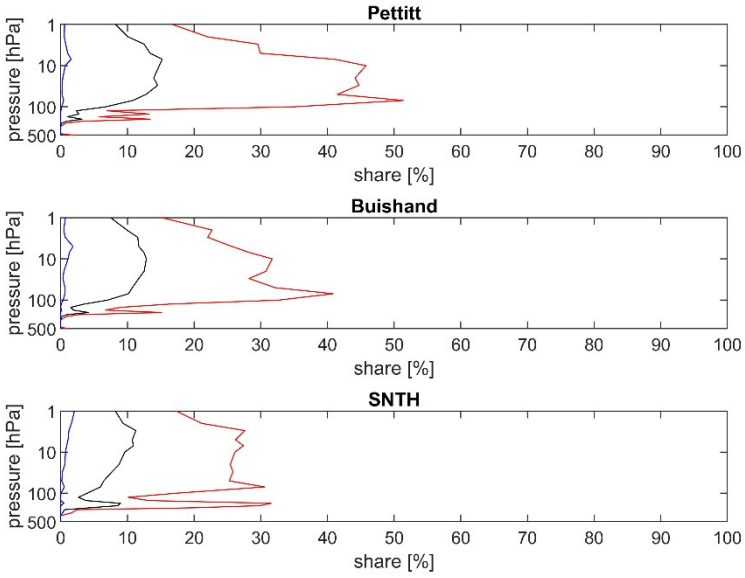


Figure S14. The same as Figure S13, but for JRA-55.

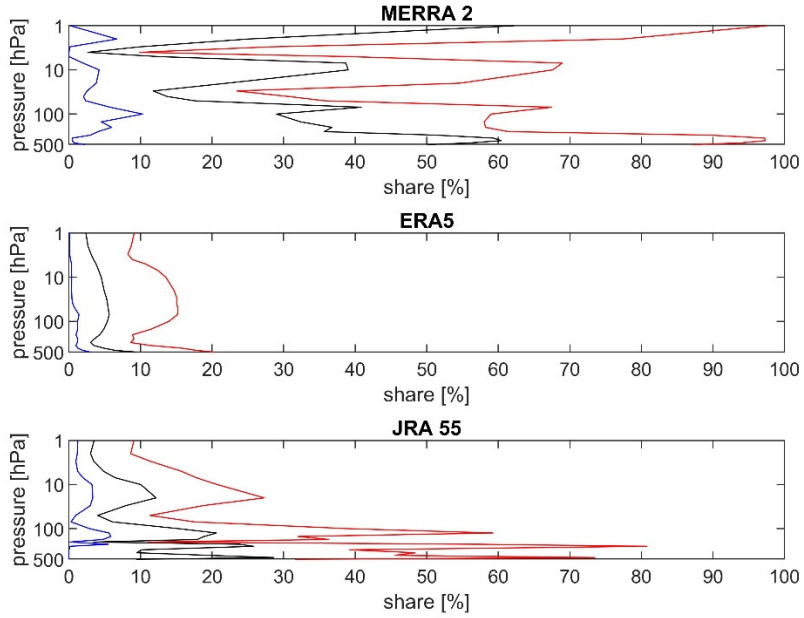


Figure S15. The same as Figure S15, but for the Standard homogeneity test.

Table S1. Minimal, average, and maximal share of discontinuities in percentage to all grids from all months from ERA-5 for the Pettitt test, the Buishand test, and the Standard Normal Homogeneity test.

ERA-5	Pettitt	Buishand	Standard
minimum	34.2	46.4	53.7
average	48.1	61.5	72.0
maximum	64.4	72.5	83.3

Table S2. The same as Table S1, but for JRA-55.

JRA-55	Pettitt	Buishand	Standard
minimum	27.6	33.3	31.5

average	37.5	42.8	41.2
maximum	46.2	52.3	49.9

Table S3. Minimal, average and maximal share of discontinuities in percentage to all discontinuities in 2003/2004/2005 from ERA-5 for the Pettitt test, the Buishand test and the Standard Normal Homogeneity test.

ERA-5	Pettitt	Buishand	SNTH
minimum	1.3/1.4/0.7	1.1/0.8/1.1	0.6/0.5/0.4
average	6.4/5.1/4.4	5.7/4.8/4.5	3.1/3.0/2.8
maximum	13.3/13.3/12.7	11.3/11.3/12.2	7.0/7.5/6.6

Table S4. The same as Table S3, but for JRA-55.

JRA-55	Pettitt	Buishand	SNTH
minimum	0.2/0.3/0.0	0.3/0.4/0.1	0.0/0.2/0.0
average	2.0/6.5/1.0	2.0/5.9/1.2	1.1/4.2/1.1
maximum	5.5/20.3/4.1	5.3/16.5/5.0	3.6/13.8/4.6

Table S5. Minimal, average and maximal share of discontinuities in percentage to all discontinuities in 2014/2015/2016 from ERA-5 for the Pettitt test, the Buishand test and the Standard Normal Homogeneity test.

ERA-5	Pettitt	Buishand	SNTH
minimum	0/0/0	0/0/0	0.3/0.2/0.0
average	0/0/0	1.0/0.0/0	7.5/1.9/2.4
maximum	0/0/0	10.0/0.0/0	26.6/7.4/12.8

Table S6. The same as Table S5, but for JRA-55.

JRA-55	Pettitt	Buishand	SNTH
minimum	0/0/0	0/0/0	0.0/0/0
average	0/0/0	0.0/0/0	0.5/1.4/0.2
maximum	0/0/0	0.0/0/0	1.7/6.5/2.1

Table S7. Minimal, average, and maximal share of explained discontinuities in percentage by the change in 2004 to all discontinuities from all months from ERA-5 for the Pettitt test, the Buishand test, and the Standard Normal Homogeneity test.

ERA-5	Pettitt	Buishand	Standard
minimum	1.4	0.8	0.5
average	5.1	4.8	3.0
maximum	13.3	11.3	7.5

Table S8. The same as Table S7, but for JRA-55.

JRA-55	Pettitt	Buishand	Standard
minimum	0.3	0.4	0.2
average	6.5	5.9	4.2
maximum	20.3	16.5	13.8

Table S9. Minimal, average, and maximal share in percentage of explained discontinuities by the change in 2015 to all discontinuities from all months from ERA-5 for the Pettitt test, the Buishand test, and the Standard Normal Homogeneity test. 0 means mathematical zero, 0.0 nearly zero, but not mathematical zero.

ERA-5	Pettitt	Buishand	Standard
minimum	0	0	0.2
average	0	0.0	1.9
maximum	0	0.0	7.4

Table S10. The same as Table S5, but for JRA-55.

JRA-55	Pettitt	Buishand	Standard
minimum	0	0	0
average	0	0	1.4
maximum	0	0	6.5

Table S11. Minimal, average, and maximal share of explained discontinuities in percentage by the change in 2004 and in 2015 to all discontinuities from all months from ERA-5 for the Pettitt test, the Buishand test, and the Standard Normal Homogeneity test.

ERA-5	Pettitt	Buishand	Standard
minimum	1.4	0.8	1.9
average	5.1	5.8	10.4
maximum	13.2	19.2	31.3

Table S12. The same as Table S6, but for JRA-55.

JRA-55	Pettitt	Buishand	Standard
minimum	0.3	0.4	0.4
average	6.5	5.9	5.5
maximum	20.3	16.5	17.2

Now we describe in detail the homogeneity tests used in this paper. Suppose we have a time series, which consists of independent members with normal distribution with the length 10: $X_1 \ldots X_{10}$. This time series is displayed in the second row of Table S13. We see there is a discontinuity between the 5th and 6th member.

Buishand test

At first we compute the average and the standard deviation of series X_{avg} and σ. In our series the average is 55 and the standard deviation is 47.4. Next we compute the cumulative sum of deviations from mean divided by the standard deviation:

$$b = \sum_{x=1}^{n} (Xi - Xavg)/\sigma \qquad (S1)$$

The values of this sum are given at the third row of table S13. Then we find the maximum in absolute value from these sums and this the statistic of the Buishand test. In our case it is 4.74 and it is situated in 5th member of series, where the discontinuity is observed. This maximal value is then divided by $n^{1/2}$ We must find if this value is significant. If it is above a certain threshold, we reject the null hypothesis that there is no discontinuity in the series. Otherwise, we are not able to reject the null hypothesis. The threshold statistic values for various significance levels and various length of series is given in Table S14. Our maximal value is 1.50, which is above the threshold value from Table S14(1.14 for n=10). In the last row of Table S13 the absolute maximal values of cumulative sums divided by $n^{1/2}$ are given when we move with the position of discontinuity forward or backward. The maximal values are observed when the discontinuity is situated in the middle of series. It means the Buishand test has the best performance when the discontinuity is situated in the middle of series.

Table S13. Values of series (second row), cumulative sum of deviations from mean divided by standard deviations (third row) and the absolute maximal values of test statistic (fourth row)

	1	2	3	4	5	6	7	8	9	10
member	10	10	10	10	10	100	100	100	100	100
cumsum	−0.95	−1.90	−2.84	−3.79	−4.74	−3.79	−2.84	−1.90	−0.95	0
statistic	0.88	1.20	1.38	1.47	1.50	1.47	1.38	1.20	0.88	0

Table S14. Threshold values of statistic for the Buishand test for various significance level and various length of time series.

	10	20	30	40	50	100
1%	1.29	1.42	1.46	1.50	1.52	1.55
5%	1.14	1.22	1.24	1.26	1.27	1.29

Pettitt test

Again we have the same series $x_1 \ldots x_{10}$. The Pettitt test used the following statistic:

$$U_{t_iT}=\sum_{i=1}^{t}\sum_{j=t+1}^{T}D_{ij} \quad (S2)$$

where

$$D_{ij}=\mathrm{sgn}(X_i-X_j)=\begin{cases}-1 & (X_i-X_j)<0\\ 0 & (X_i-X_j)=0\\ +1 & (X_i-X_j)>0\end{cases}$$

The values of statistic $U_{t,T}$ are given in the second row of Table S15 for each member of the series. We find the maximal value of $U_{t,T}$ in absolute value. It is the 5th member of the series. We must search if this value is suitable for rejecting the null hypothesis, that there is no discontinuity in the series. For this reason, we compute the probability of null hypothesis according the following formula:

$$P=\exp(-6K_T^2/(T^2+T^3)) \quad (S3)$$

Where K_T is the maximal value of $U_{t,T.}$ In our case K_T=25 and T is the length of series (10) After substituting these values to (S3) we obtain the propability of null hypothesis 0.032, which is lower than 0.05 and so we can reject the null hypothesis at the 0.05 level. In the last row of the Table S15 the values of K_T are showed when we move with the position of discontinuity backward or forward. We see the maximal values of K_T where the discontinuity is situated in the middle of series.

Table S15. Values of series (second row), Ut,T statistic (third row) and KT (fourth row)

	1	2	3	4	5	6	7	8	9	10
member	10	10	10	10	10	100	100	100	100	100
$U_{t,T}$	−5	−10	−15	−20	−25	−20	−15	−10	−5	0
K_T	−9	−16	−21	−24	−25	−24	−21	−16	−9	0

Standard Homogeneity test

Again we have our series $x_1 \ldots x_{10}$. We compute its average and standard deviation. In Standard test we have the following statistic, which compares the mean of the first k observations with the mean of the remaining (n – k) observations:

$$T(k) = kz_1^2 + (n-k)z_2^2 \quad k = 1, \ldots, n \quad (S4)$$

where

$$Z_1=(1/k)\sum_{i=1}^{k}(x_i-x_{avg})/\sigma \qquad Z_2=(1/k)\sum_{i=k+1}^{n}(x_i-x_{avg})/\sigma$$

The values of T_k are given at the second row of Table S16. We look for maximal value of this statistic. We see this maximal value is 8.1 for our series. If this statistic is above certain value, we reject the null hypothesis that there is no discontinuity in series. The threshold values are given in Table S17. From this table we see we can reject the null hypothesis. In the last row of Table S16 we see the maximal value of T_k, where we shift the position of discontinuity backward or forward. The maximal values are observed when the discontinuity is situated at the beginning of series. When we approach to the end of series the values of T_k decreases.

Table S16. Values of series (second row), T_k statistic (third row) and maximal value of T_k when we shift with the discontinuity (fourth row)

	1	2	3	4	5	6	7	8	9	10
member	10	10	10	10	10	100	100	100	100	100
T_k	1.0	2.2	3.7	5.6	8.1	5.1	3.0	1.4	0.1	
Max T_k	8.9	8.8	8.6	8.4	8.1	7.7	6.9	4.9	2.1	

Table S17. Threshold values of statistic for the Standard homogeneity test for various significance level and various length of time series.

	20	30	40	50	70	100
1%	9.56	10.45	11.01	11.38	11.89	12.32

5%	6.95	7.65	8.10	8.45	8.80	9.15