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OMI air-quality monitoring over the Middle East – Supplementary Material

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1 Introduction

This supplementary material contains additional figures and tables to support the analysis described in the main text. It is structured as follows. Section 2 contains the supporting figures, whilst Section 3 contains tabulated statistics. Tables S2 to S4 showing the results of the sensitivity analysis conducted in Section 5 of the main text. The sensitivity tests are numbered in correspondence to their descriptions in the manuscript.

2 Ancillary Figures

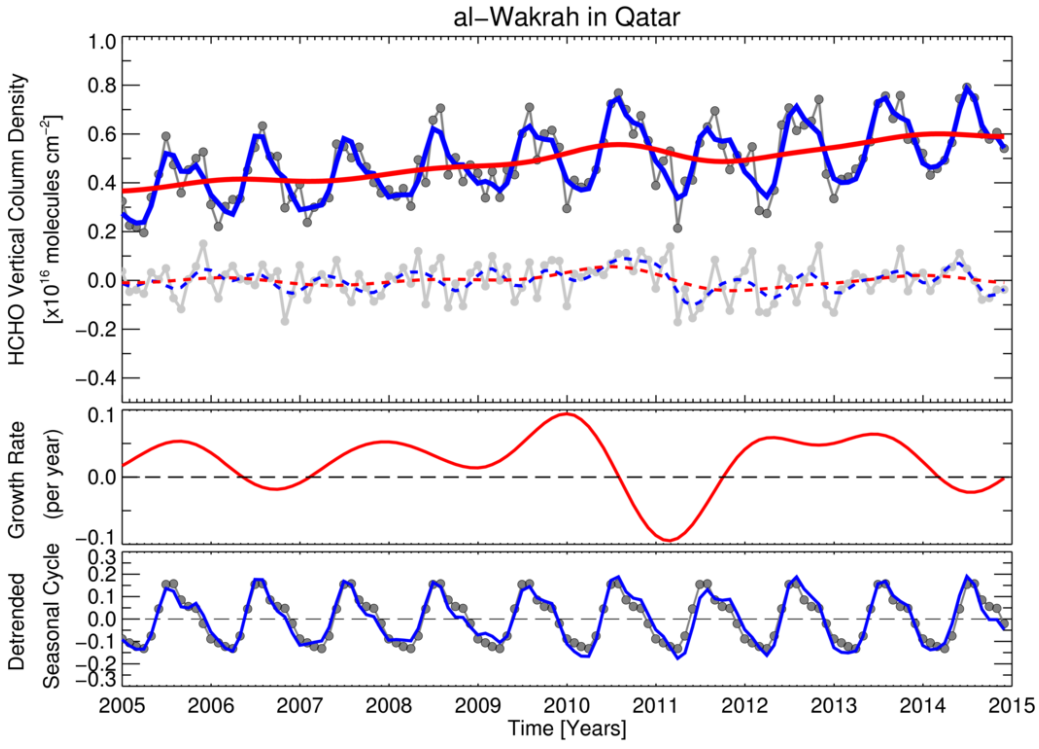

Figure 1. An example of a time series fit to observed HCHO data over al-Wakrah (Qatar), as outlined in Section 3.3. Top panel: the monthly OMI HCHO vertical columns are indicated by dark grey filled circles, whilst the light grey filled circles represent the fitting residual, which has been smoothed with a short-term 200-day filter (dashed blue line) and long-term 667-day filter (red dashed line). The solid red line is the long-term trend $F_T(t)$, given by the linear component of the fitted function $F(t)$ (equation 1) plus the residual filtered using the long-term filter. The solid blue line is the smoothed fitted curve $F_S(t)$ given by $F(t)$ plus the residual filtered using the short-term filter. Middle panel: The HCHO vertical column growth rate in 10^{16} molecules cm^{-2} yr^{-1}, which is the derivative of the long-term trend $F_T(t)$ shown in the top-panel. Bottom panel: the de-trended seasonal cycle $F_C(t)$ which is the difference between the long-term trend and the smoothed function fit (i.e. $F_S(t) - F_L(t)$). It represents the annual seasonal oscillation with any long-term trend removed. The dark grey filled circles are the fitted harmonic component of $F(t)$. At al-Wakrah (25.29°N, 51.61°E, population: 22712) there is a statistically significant large upward linear trend of 0.22±0.05 $\times 10^{15}$ molecules cm^{-2} yr^{-1}. This corresponds to a linear growth of 4.61±0.94 % yr^{-1} relative to the observed 2005–2014 median VCD. In this example, $|\omega/\sigma_\omega| = 4.9$ and the uncertainties of the trend (F_T) and smoothed curves (F_S) are about 4% and 6%, respectively. The median growth rate G is 6.56±5.61 % yr^{-1}, whilst the mean seasonal amplitude is 3.05±0.36 $\times 10^{15}$ molecules cm^{-2} (about 62.56±7.36% relative to the median column). A similar analysis of the coincident time series of the HCHO AMF, cloud fraction, cloud-top pressure and number of samples, reveals no other significant trend. This indicates the upward growth in HCHO is not caused by a trend in any other retrieval parameter and is real at the 95% confidence level.

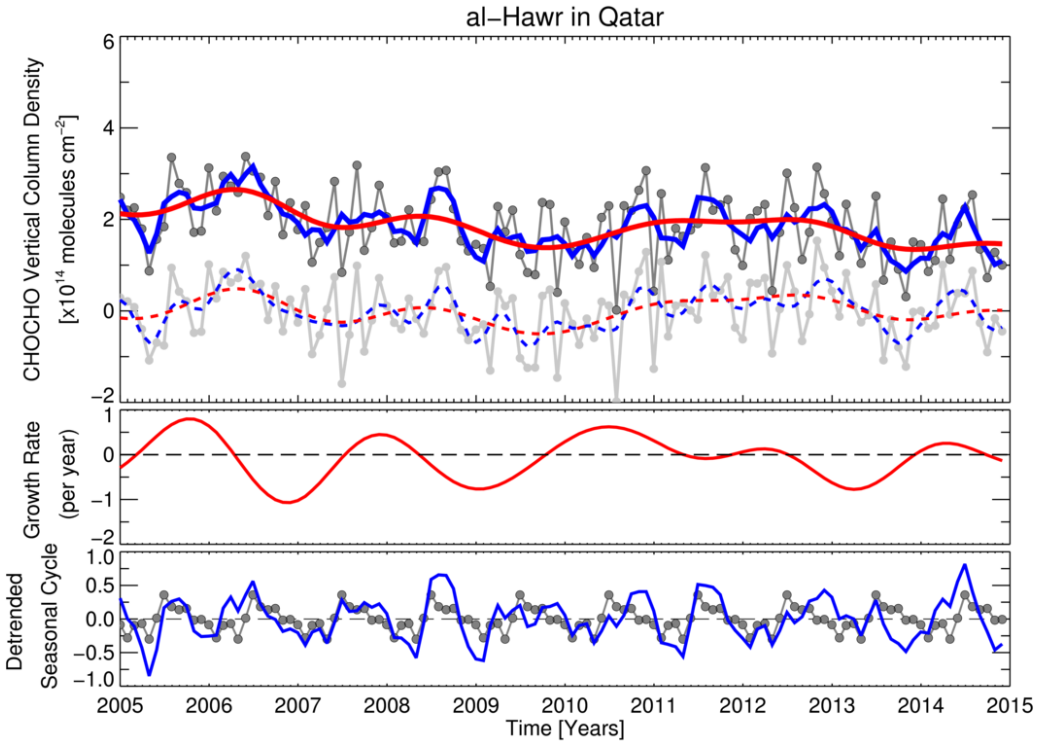

Figure 2. An example of a time series fit to observed CHOCHO data over al-Hawr (Qatar), as outlined in Section 3.3. Top panel: the monthly OMI CHOCHO vertical columns are indicated by dark grey filled circles, whilst the light grey filled circles represent the fitting residual, which has been smoothed with a short-term 200-day filter (dashed blue line) and long-term 667-day filter (red dashed line). The solid red line is the long-term trend $F_T(t)$, given by the linear component of the fitted function $F(t)$ (equation 1) plus the residual filtered using the long-term filter. The solid blue lines is the smoothed fitted curve $F_S(t)$ given by $F(t)$ plus the residual filtered using the short-term filter. Middle panel: The CHOCHO vertical column growth rate in 10^{14} molecules cm^{-2} yr^{-1}, which is the derivative of the long-term trend $F_T(t)$ shown in the top-panel. Bottom panel: the de-trended seasonal cycle $F_C(t)$ which is the difference between the long-term trend and the smoothed function fit (i.e. $F_S(t) - F_L(t)$). It represents the annual seasonal oscillation with any long-term trend removed. The dark grey filled circles are the fitted harmonic components of $F(t)$. At al-Hawr (25.69°N, 51.51°E, population: 2736) there is a statistically significant downward linear trend of -0.83 ± 0.23 $\times10^{13}$ molecules cm^{-2} yr^{-1}. This corresponds to a linear decrease of -4.58 ± 1.26 % yr^{-1} relative to the observed 2005–2014 median VCD. In this example, $|\omega/\sigma_\omega| = 2.0$ and the uncertainties of the trend (F_T) and smoothed curves (F_S) are about 10% and 16%, respectively. The median growth rate G is -0.89 ± 13.88 % yr^{-1}, whilst the mean seasonal amplitude is 9.50 ± 3.35 $\times10^{13}$ molecules cm^{-2} (about 52.12 ± 18.41% relative to the median column). A similar analysis of the coincident time series of the CHOCHO AMF, cloud fraction, cloud-top pressure and number of samples, reveals no other significant trend. This indicates the downward trend in CHOCHO is not caused by a trend in any other retrieval parameter and is real at the 95% confidence level.

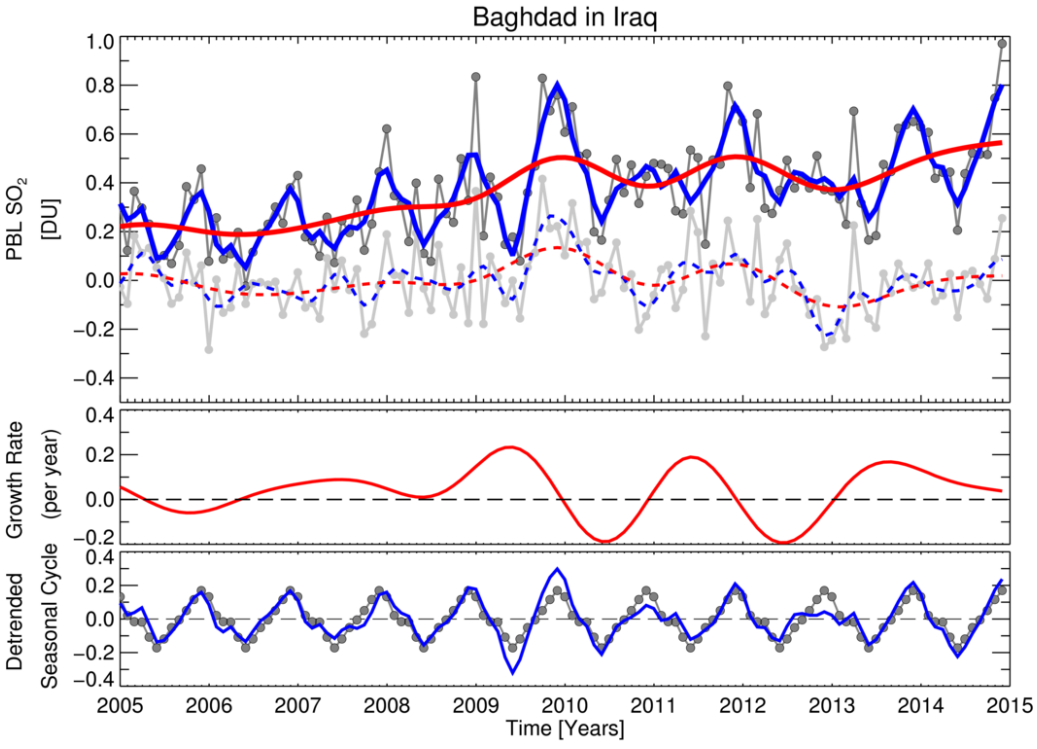

Figure 3. An example of a time series fit to observed SO_2 data over Baghdad (Iraq), as outlined in Section 3.3. Top panel: the monthly OMI SO_2 vertical columns are indicated by dark grey filled circles, whilst the light grey filled circles represent the fitting residual, which has been smoothed with a short-term 200 day filter (dashed blue line) and long-term 667 day filter (red dashed line). The solid red line is the long-term trend $F_T(t)$, given by the linear component of the fitted function $F(t)$ (equation 1) plus the residual filtered using the long-term filter. The solid blue line is the smoothed fitted curve $F_S(t)$ given by $F(t)$ plus the residual filtered using the short-term filter. Middle panel: The SO_2 vertical column growth rate in DU yr^{-1}, which is the derivative of the long-term trend $F_T(t)$ shown in the top-panel. Bottom panel: the de-trended seasonal cycle $F_C(t)$ which is the difference between the long-term trend and the smoothed function fit (i.e. $F_S(t) - F_L(t)$). It represents the annual seasonal oscillation with any long-term trend removed. The dark grey filled circles are the fitted harmonic components of $F(t)$. At Baghdad (33.34°N, 44.39°E, population: 5511490) there is a statistically significant large upward linear trend of 0.035±0.008 DU yr^{-1}. This corresponds to a linear growth of 9.78±2.25 % yr^{-1} relative to the observed 2005–2014 median VCD. In this example, $|\omega/\sigma_\omega| = 4.4$ and the uncertainties of the trend (F_T) and smoothed curves (F_S) are about 9% and 15%, respectively. The median growth rate G is 13.18±13.37 % yr^{-1}, whilst the mean seasonal amplitude is 0.37±0.06 DU (about 102.78±17.78% relative to the median column). A similar analysis of the coincident time series of the SO_2 cloud fraction, cloud-top pressure and number of samples, reveals no other significant trend. This indicates the upward growth in SO_2 is not caused by a trend in any other retrieval parameter and is real at the 95% confidence level.

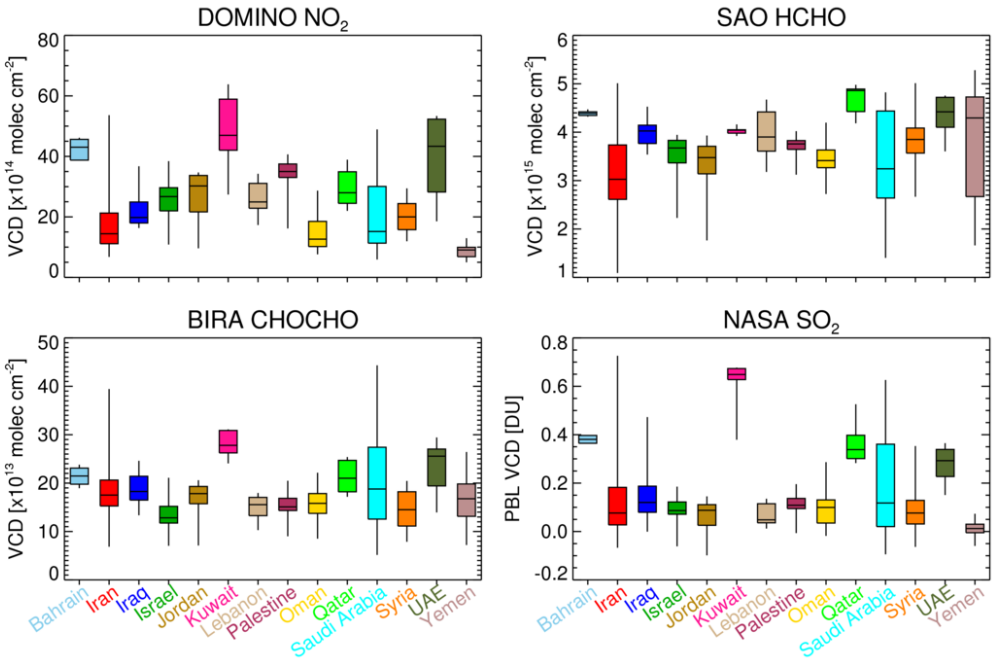

Figure 4. Box-and-whisker plots showing the minimum, 25th percentile, median, 75th percentile, and maximum values of the observed median vertical columns, for urban targets categorised by country.

3 Statistical Summaries

Table 3. The difference between the linear trend (in % yr^{-1}) and inferred growth rates (in % yr^{-1}) per species and target category.

Species	Urban	Refinery	Ports	Plants
NO_2				
Maximum	4.84	3.18	2.49	4.21
Minimum	−5.29	−1.56	−0.95	−4.90
Median	−0.18	−0.09	−0.11	0.78
HCHO				
Maximum	3.42	1.33	1.10	3.42
Minimum	−2.46	0.00	−0.70	−2.34
Median	−0.06	0.90	0.08	−0.93
SO_2				
Maximum	31.50	5.66	6.03	77.06
Minimum	−21.63	−2.44	−0.36	−16.63
Median	0.21	−0.97	2.84	0.33
CHOCHO				
Maximum	−3.69	–	–	3.14
Minimum	−3.69	–	–	3.14
Median	−3.69	–	–	3.14

Table 4. Statistical summary of the DOMINO NO_2 vertical column density (VCD) analysis. Tests 1–6 are defined as follows: (1) construction of each 10 year time series using mask of ± 4 grid-cells ($\sim$20 km radius around each target), instead of the default ± 2 grid-cells ($\sim$10 km radius around each target), (2) use of cloud fraction filter of 40%, (3) use of unaffected OMI detector rows 5 to 23 only, (4) increased smoothing of gridded maps (spatial filter of $0.35^\circ \times 0.35^\circ$ with a 2-σ width), (5) no filtering for outliers in the time series analysis, (6) focus on only locations with >500,000 people using a spatial mask of ± 16 grid-cells ($\sim$80 km radius around each target). Column headers are: n=number of locations with trends, n_{same} number of same locations with trends as found in default analysis, n_{new}= number of new locations trend found in the this test, and n_{miss} is the number of locations from the original analysis that have not been detected.

Test	Urban Targets (default=198)				Refinery default=17				Oil Ports default=6				Power Plants default=57			
	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}
Test 1	220	170	50	28	17	14	3	3	6	5	1	1	69	51	18	6
Test 2	165	159	6	39	13	13	0	4	6	6	0	0	49	43	6	14
Test 3	95	57	38	141	6	4	2	13	5	3	2	3	30	14	16	43
Test 4	207	194	13	4	15	15	0	2	6	6	0	0	59	56	3	1
Test 5	199	172	27	26	16	15	1	2	6	6	0	0	58	52	6	5
Test 6	22	12	10	186	–	–	–	–	–	–	–	–	–	–	–	–

Table 5. Statistical summary of the SAO HCHO vertical column density (VCD) analysis. Tests 1–6 are defined as follows: ((1) construction of each 10 year time series using mask of ± 4 grid-cells ($\sim$20 km radius around each target), instead of the default ± 2 grid-cells ($\sim$10 km radius around each target), (2) use of cloud fraction filter of 40%, (3) use of unaffected OMI detector rows 5 to 23 only, (4) increased smoothing of gridded maps (spatial filter of $0.35^\circ \times 0.35^\circ$ with a 2-σ width), (5) no filtering for outliers in the time series analysis, (6) focus on only locations with >500,000 people using a spatial mask of ± 16 grid-cells ($\sim$80 km radius around each target).. Column headers are: n=number of locations with trends, n_{same} number of same locations with trends as found in default analysis, n_{new}= number of new locations trend found in the this test, and n_{miss} is the number of locations from the original analysis that have not been detected.

Test	Urban Targets (default=34)				Refinery default=6				Oil Ports default=4				Power Plants default=26			
	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}
Test 1	46	29	17	5	7	6	1	0	8	4	4	0	34	21	13	5
Test 2	34	27	7	7	3	3	0	3	4	3	1	1	27	22	5	4
Test 3	19	7	12	27	4	3	1	3	1	1	0	3	14	10	4	16
Test 4	43	33	10	1	6	6	0	0	5	4	1	0	33	26	7	0
Test 5	33	31	2	3	6	6	0	0	4	4	0	0	29	25	4	1
Test 6	9	3	6	31	–	–	–	–	–	–	–	–	–	–	–	–

Table 6. Statistical summary of the NASA SO_2 vertical column density (VCD) analysis, tests 1–6 are defined as follows: (1) construction of each 10 year time series using mask of ± 4 grid-cells ($\sim$20 km radius around each target), instead of the default ± 2 grid-cells ($\sim$10 km radius around each target), (2) use of cloud fraction filter of 40%, (3) use of unaffected OMI detector rows 5 to 23 only, (4) increased smoothing of gridded maps (spatial filter of $0.35^\circ \times 0.35^\circ$ with a 2-σ width), (5) no filtering for outliers in the time series analysis, (6) focus on only locations with >500,000 people using a spatial mask of ± 16 grid-cells ($\sim$80 km radius around each target).. Note that test 2 (different cloud fraction filtering) was not applied to the SO_2 data. Column headers are: n=number of locations with trends, n_{same} number of same locations with trends as found in default analysis, n_{new}= number of new locations trend found in the this test, and n_{miss} is the number of locations from the original analysis that have not been detected.

Test	Urban Targets (default=18)				Refinery (default=3)				Oil Ports (default=2)				Power Plants (default=9)			
	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}
Test 1	18	9	9	9	3	3	0	0	3	1	2	1	9	6	3	3
Test 3	13	8	5	10	1	1	0	2	1	1	0	1	10	5	5	4
Test 4	17	17	0	1	3	3	0	0	3	2	1	0	9	8	1	1
Test 5	14	11	3	7	2	2	0	1	1	1	0	1	4	3	1	6
Test 6	3	1	2	17	–	–	–	–	–	–	–	–	–	–	–	–

Table 7. Statistical summary of the BIRA CHOCHO vertical column density (VCD) analysis, tests 1–5 are defined as follows: (1) construction of each 10 year time series using mask of ± 4 grid-cells ($\sim$20 km radius around each target), instead of the default ± 2 grid-cells ($\sim$10 km radius around each target), (2) use of cloud fraction filter of 40%, (3) use of unaffected OMI detector rows 5 to 23 only, (4) increased smoothing of gridded maps (spatial filter of $0.35^\circ \times 0.35^\circ$ with a 2-σ width), (5) no filtering for outliers in the time series analysis, (6) focus on only locations with >500,000 people using a spatial mask of ± 16 grid-cells ($\sim$80 km radius around each target). Note that test 2 (different cloud fraction filtering) was not applied to the SO_2 data. Column headers are: n=number of locations with trends, n_{same} number of same locations with trends as found in default analysis, n_{new}= number of new locations trend found in the this test, and n_{miss} is the number of locations from the original analysis that have not been detected.

Test	Urban Targets (default=1)				Refinery (default=0)				Oil Ports (default=0)				Power Plants (default=1)			
	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}	n	n_{same}	n_{new}	n_{miss}
Test 1	2	1	1	0	1	0	1	0	0	0	0	1	1	1	0	0
Test 3	2	0	2	1	0	0	0	0	0	0	0	0	0	0	0	1
Test 4	2	1	1	0	0	0	0	0	0	0	0	0	1	1	0	0
Test 5	1	0	1	0	0	0	0	0	0	0	0	0	3	1	2	0
Test 6	0	0	0	0	–	–	–	–	–	–	–	–	–	–	–	–

References

10 Kootungal, L.: 2010 WorldWide Refining Survery, Oil & Gas Journal, 6, 2010.