

Supplement of:

Formaldehyde and hydroperoxide distribution around the Arabian Peninsula – Comparison of ship-based measurements with the general circulation model EMAC

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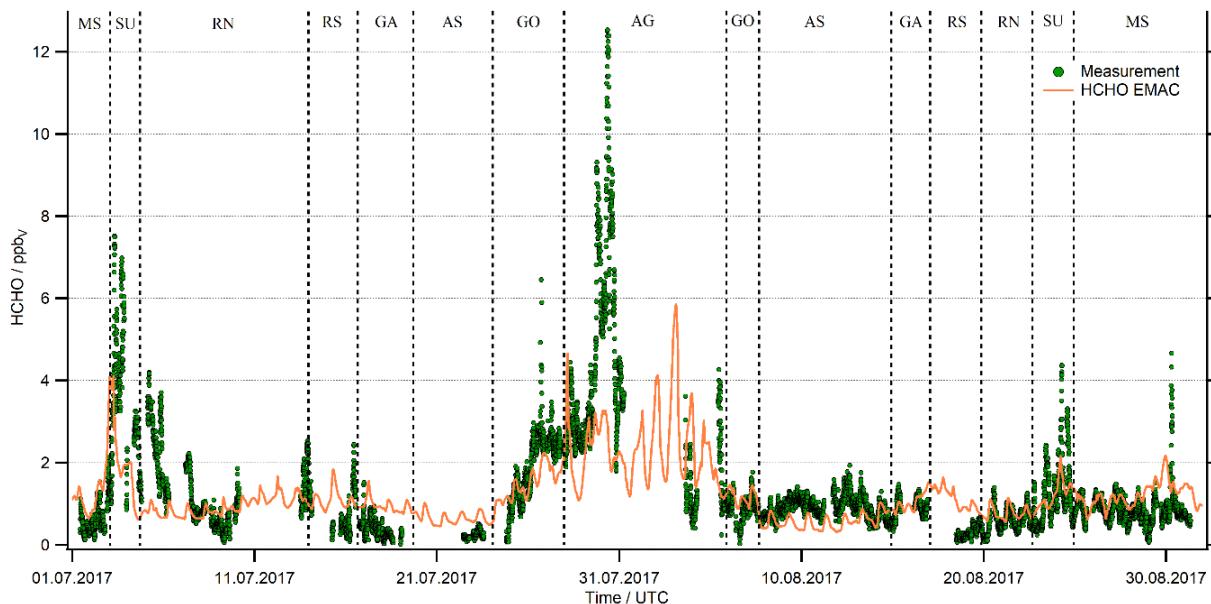


Figure S1: Timelines of the HCHO measurements and the EMAC simulation, averaged along the ship track.

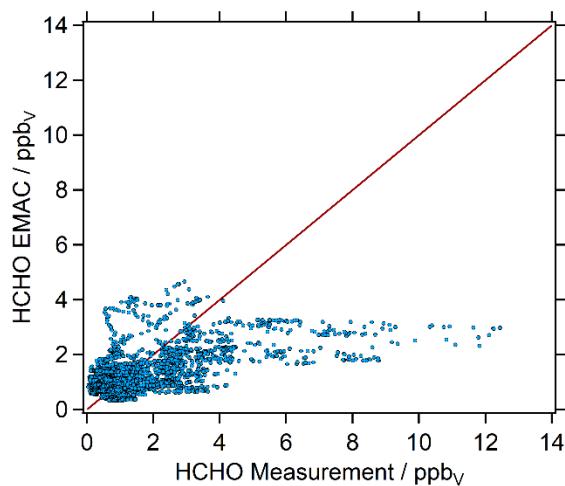


Figure S2: Scatter plot of the HCHO measurements versus the simulated data (EMAC) in hourly averages.

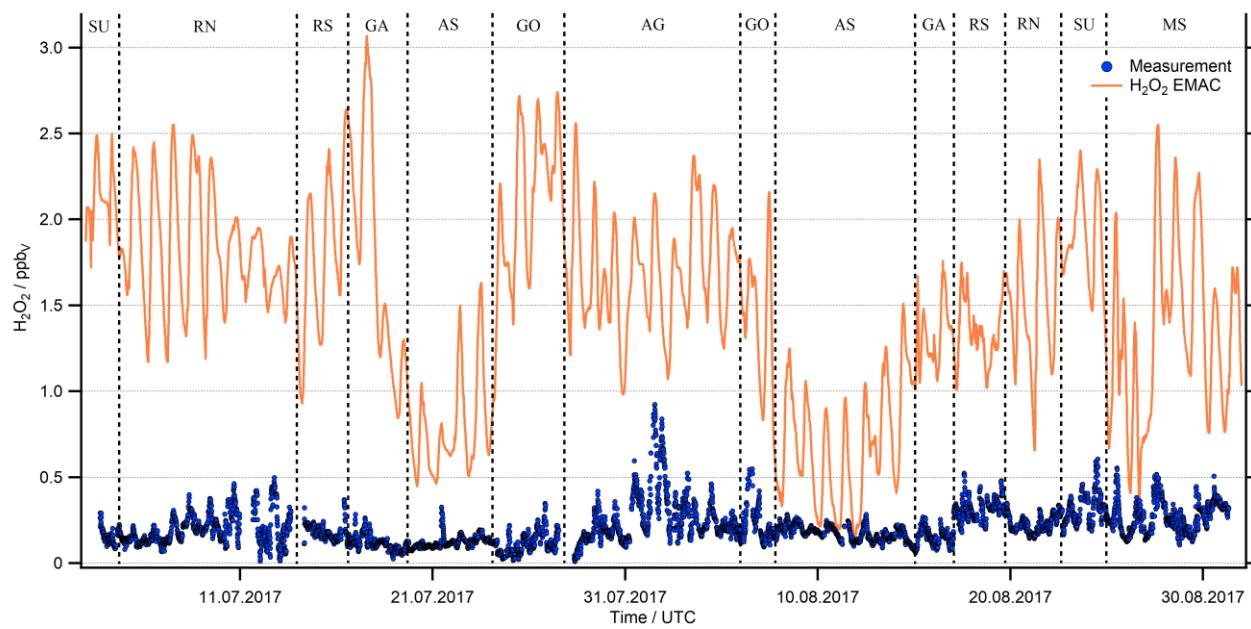


Figure S3: Timelines of the H_2O_2 measurements and the EMAC simulation, averaged along the ship track.

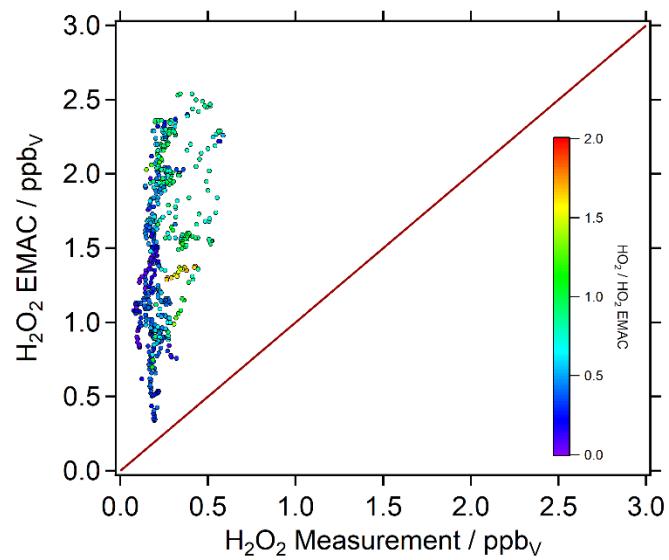


Figure S4: Scatter plot of the H_2O_2 measurements versus the simulated data (EMAC) in hourly averages.

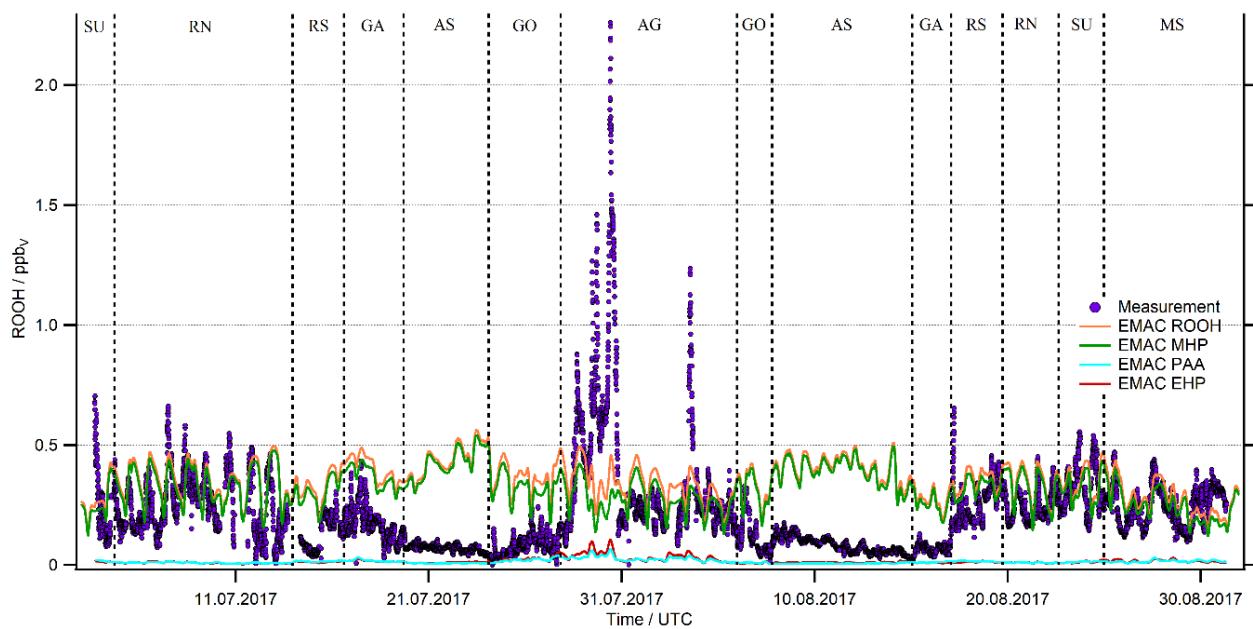


Figure S5: Timelines of the organic peroxide (ROOH) measurements and the EMAC simulations along the ship the track. The simulated dataset consists of the most prominent species methyl hydroperoxide (MHP), peracetic acid (PAA) and ethyl hydroperoxide (EHP).

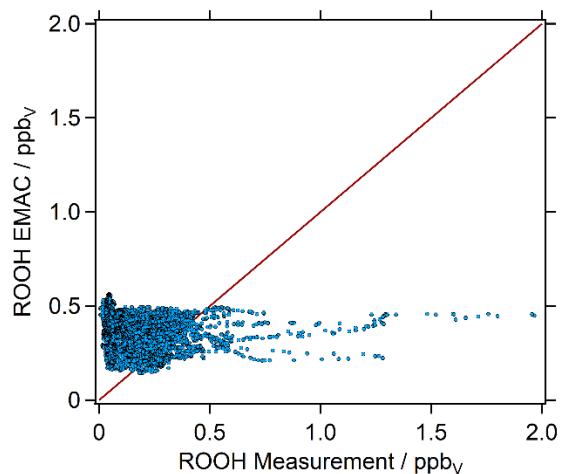


Figure S6: Scatter plot of the organic peroxide measurements versus the simulated data (EMAC) in hourly averages.

Table S1: Mean, median, 25- and 75-percentile values of the HCHO, H₂O₂ and organic peroxide measurements (black) and the corresponding EMAC simulations (orange) for the eight different regions encountered during AQABA: Mediterranean Sea (MS), Suez Canal (SU), Red Sea North (RN), Red Sea South (RS), Gulf of Aden (GA), Arabian Sea (AS), Gulf of Oman (GO) and Arabian Gulf (AG).

HCHO	MS	SU	RN	RS	GA	AS	GO	AG
Mean	0.818±0.397	2.074±1.612	1.037±0.783	0.519±0.435	0.566±0.337	0.826±0.326	1.499±0.831	3.769±2.443
±SDev	1.260±0.389	1.535±0.837	0.799±0.145	0.986±0.192	1.019±0.169	0.588±0.178	1.410±0.331	2.259±0.765
Median	0.771	1.499	0.763	0.374	0.503	0.862	1.218	3.077
	1.220	1.290	0.775	0.942	0.966	0.572	1.360	2.190
25%	0.602	0.888	0.520	0.232	0.286	0.633	0.897	2.368
	1.040	0.941	0.673	0.906	0.896	0.430	1.140	1.550
75%	0.989	2.925	1.264	0.574	0.814	1.045	2.332	4.528
	1.400	1.820	0.882	1.020	1.160	0.734	1.633	2.850
H ₂ O ₂	MS	SU	RN	RS	GA	AS	GO	AG
Mean	0.269±0.088	0.271±0.113	0.204±0.084	0.255±0.085	0.129±0.046	0.155±0.046	0.148±0.092	0.261±0.149
±SDev	1.328±0.512	1.984±0.253	1.756±0.379	1.598±0.402	1.594±0.573	0.721±0.323	1.851±0.537	1.684±0.327
Median	0.263	0.252	0.192	0.246	0.121	0.146	0.125	0.210
	1.310	2.040	1.730	1.520	1.370	0.672	1.780	1.670
25%	0.200	0.185	0.141	0.183	0.096	0.118	0.081	0.166
	0.892	1.803	1.480	1.290	1.210	0.506	1.505	1.450
75%	0.329	0.352	0.253	0.318	0.155	0.189	0.188	0.327
	1.590	2.188	1.985	1.780	1.840	0.928	2.295	1.900
ROOH	MS	SU	RN	RS	GA	AS	GO	AG
Mean	0.216±0.069	0.270±0.094	0.220±0.096	0.173±0.083	0.110±0.064	0.065±0.026	0.079±0.047	0.348±0.285
±SDev	0.276±0.074	0.325±0.066	0.351±0.082	0.345±0.051	0.355±0.077	0.419±0.059	0.347±0.066	0.335±0.075
Median	0.223	0.260	0.205	0.171	0.096	0.057	0.070	0.226
	0.261	0.315	0.366	0.344	0.349	0.419	0.357	0.335
25%	0.158	0.198	0.150	0.122	0.061	0.046	0.048	0.183
	0.221	0.266	0.290	0.305	0.289	0.375	0.295	0.291
75%	0.269	0.326	0.278	0.230	0.149	0.084	0.097	0.427
	0.322	0.384	0.420	0.390	0.436	0.460	0.390	0.387

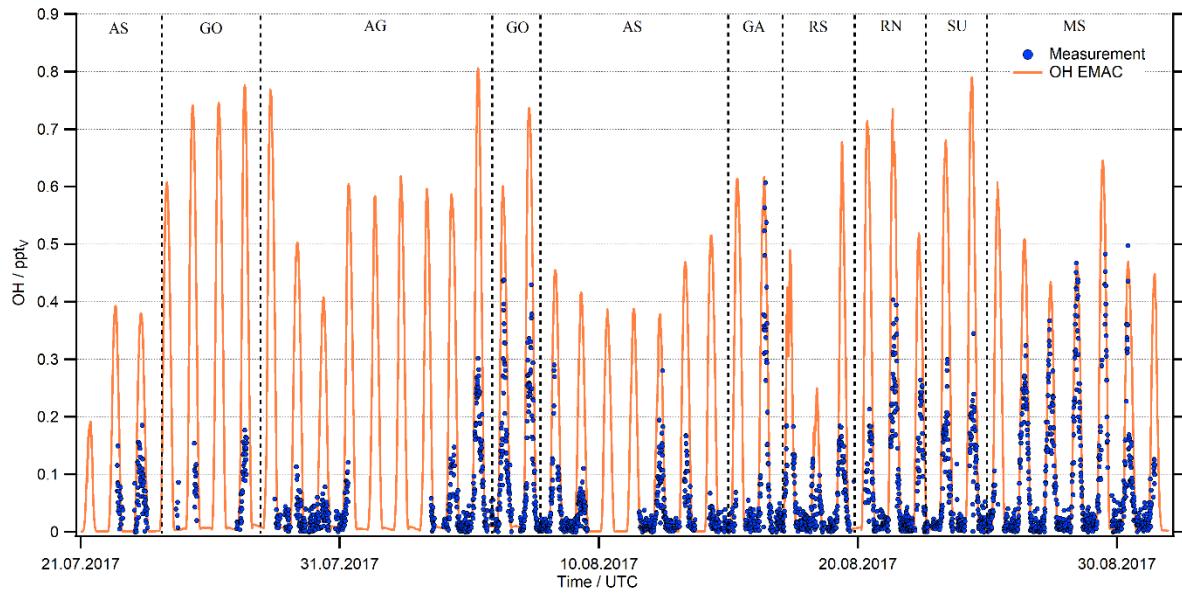


Figure S7: Timelines of the OH measurements and the EMAC simulation, averaged along the ship track.

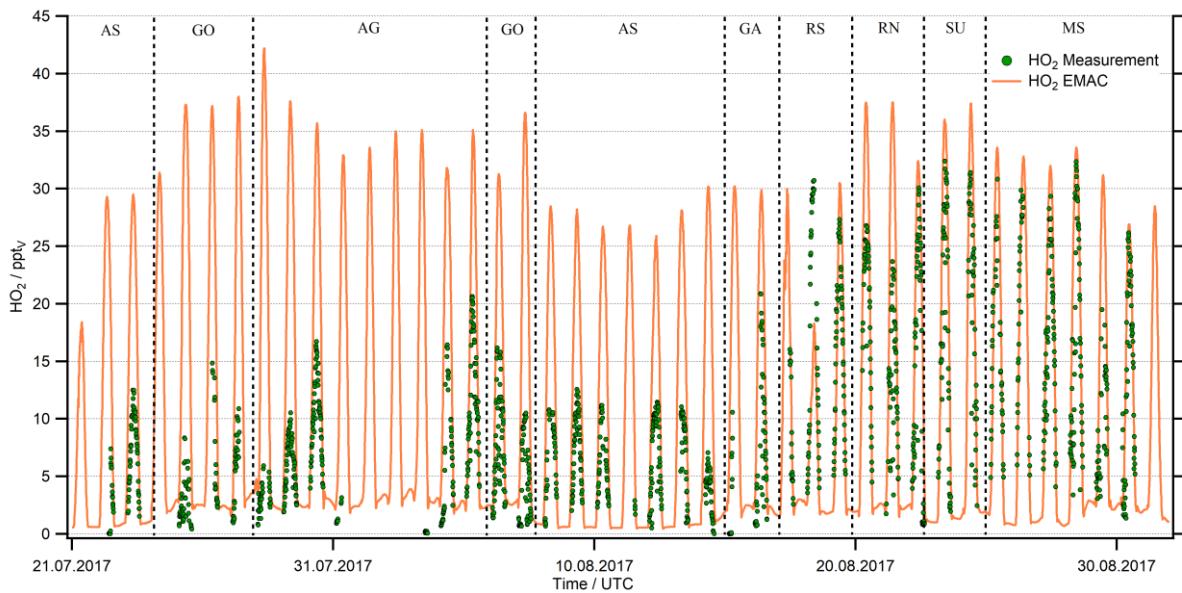


Figure S8: Timelines of the HO₂ measurements and the EMAC simulation, averaged along the ship track.

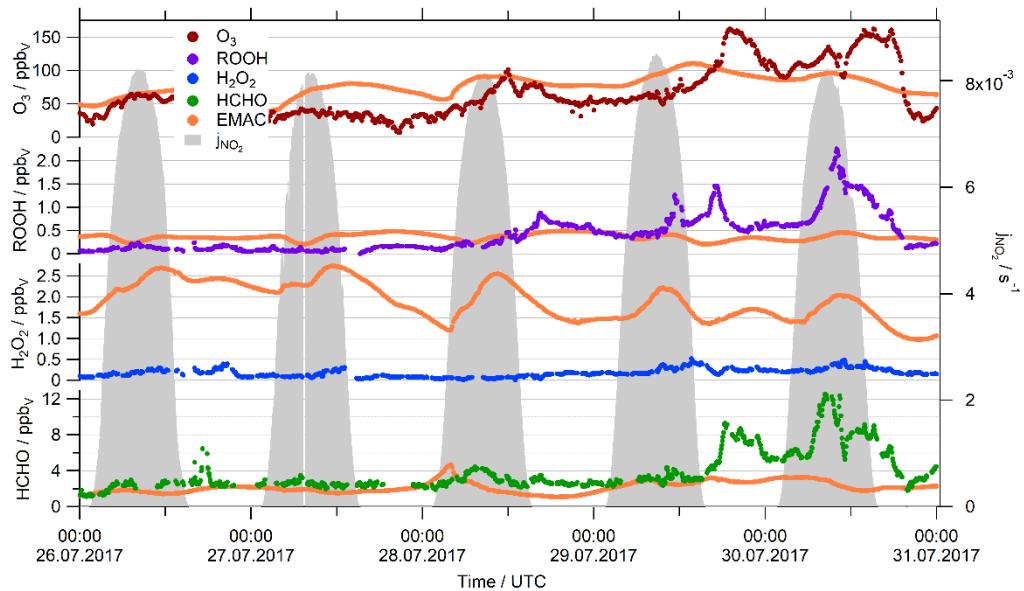


Figure S9: Case study of the Arabian Gulf during the first leg for the observations and the corresponding EMAC simulations. Highly polluted air masses were detected during the night of the 29.07.17, when we measured 170 ppbv of O₃ in the center of the Arabian Gulf.

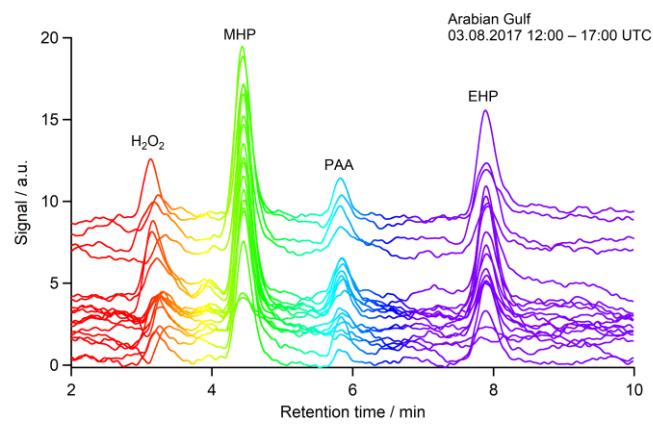
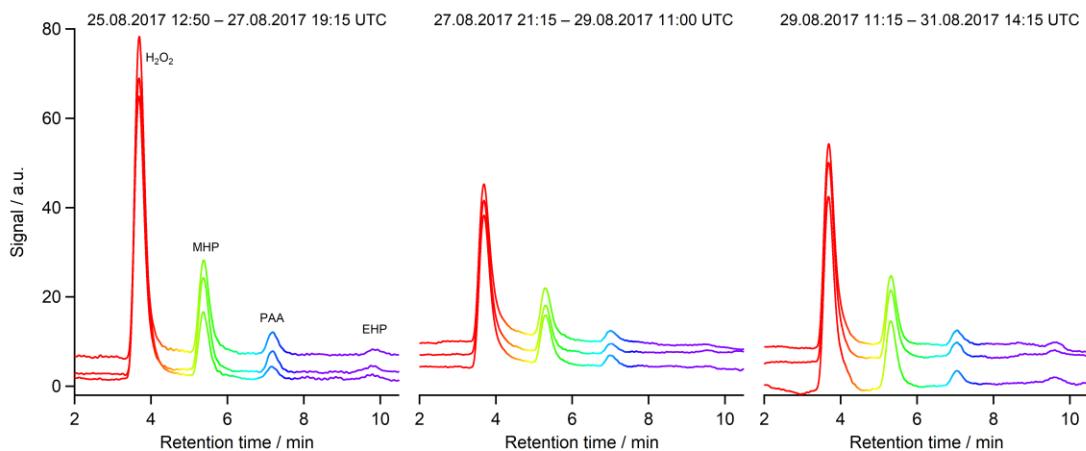


Figure S10: Identification of H₂O₂ and three separated organic peroxides based on the qualitative HPLC measurements. MHP (methyl hydroperoxide), PAA (peracetic acid) and EHP (ethyl hydroperoxide) were identified with their respective retention times and gaseous injections of PAA with a diffusion source. The lower panel shows the continuous results in AG, the upper panel the injection of enriched samples in MS.

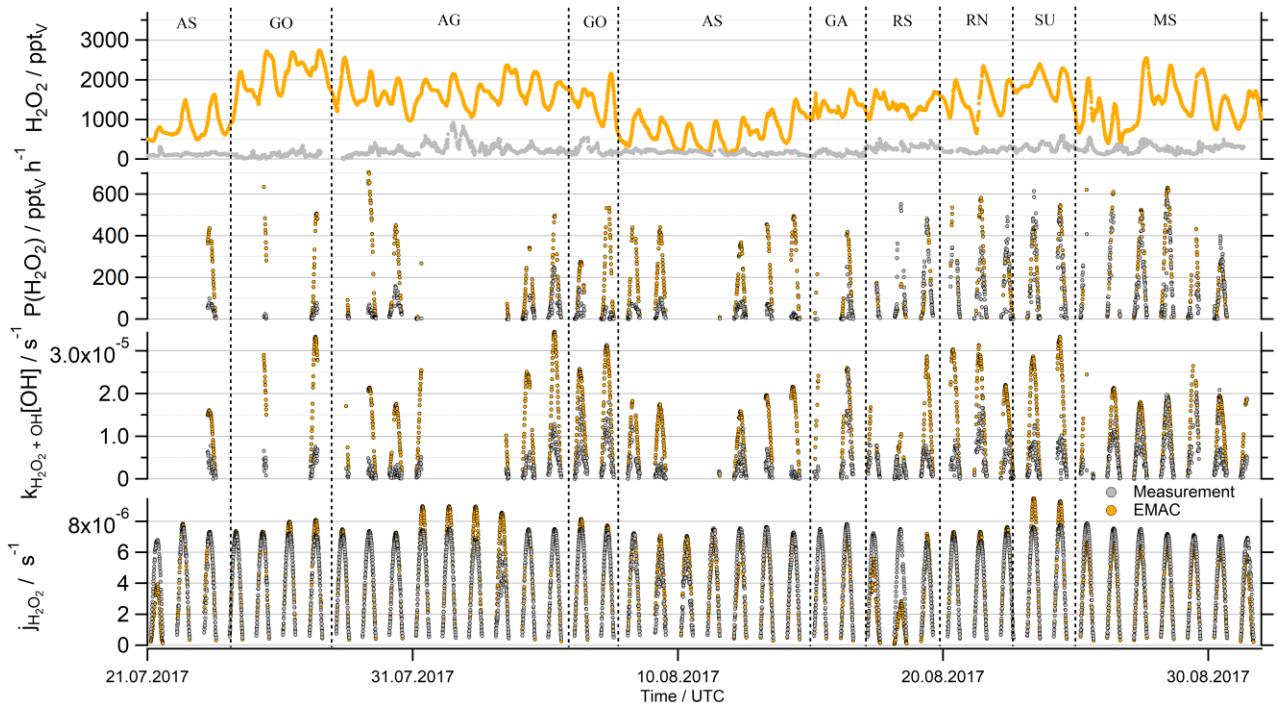


Figure S11: Timelines of the production and loss terms of H_2O_2 for the observations (black) and the EMAC model results (orange). Note that the loss terms were not multiplied with the H_2O_2 mixing ratio.

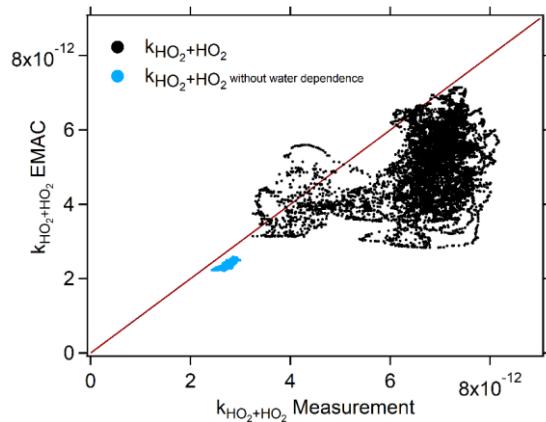


Figure S12: Scatter plot of $k_{\text{HO}_2+\text{HO}_2}$ for the measurements and EMAC. The water dependence causes a maximum deviation of about factor 2, as EMAC slightly underestimated water vapor.

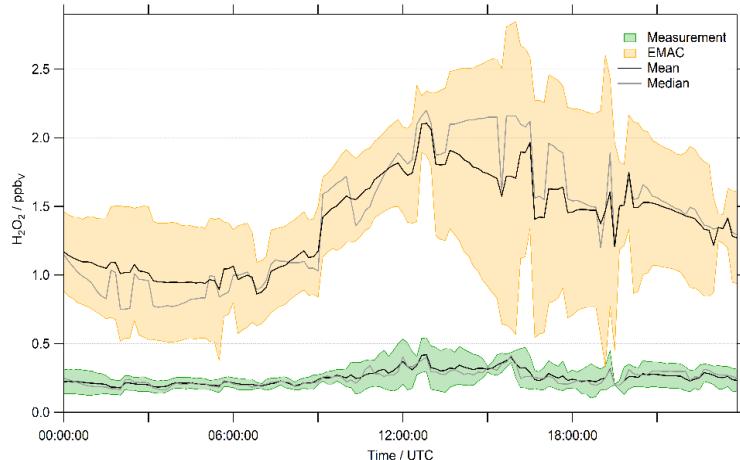


Figure S13: Diurnal variation of H_2O_2 ($\pm 1\sigma$) over the Mediterranean Sea (MS) for the observations (green) and EMAC (orange).

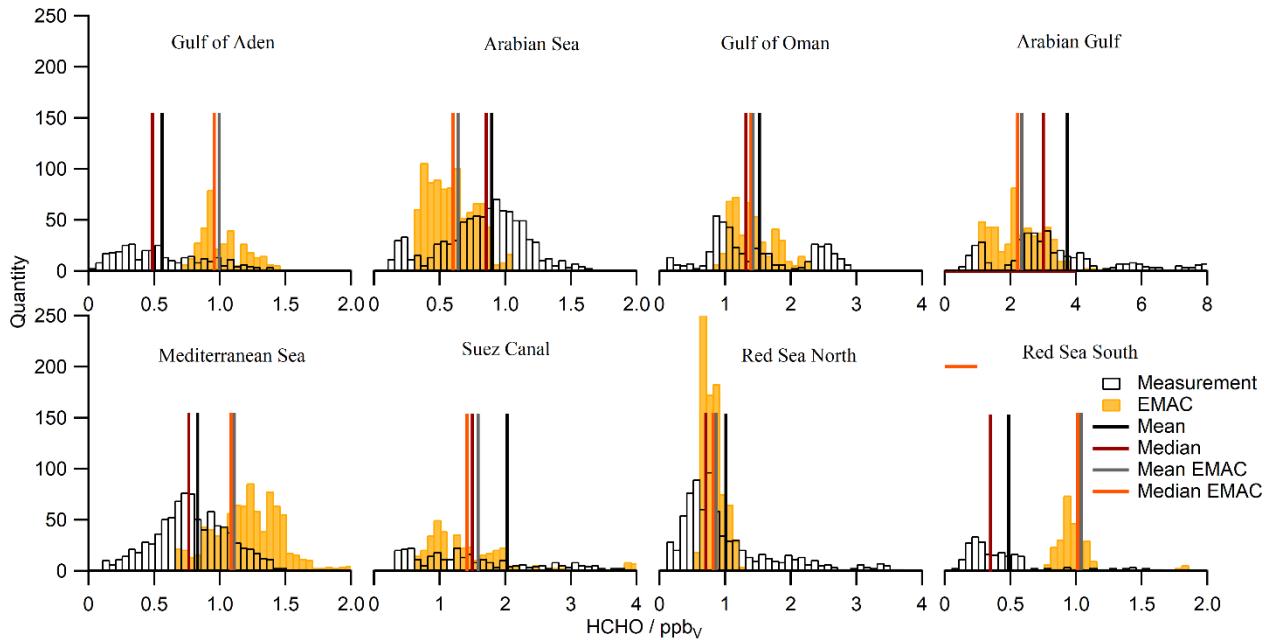


Figure S14: Frequency distributions of the HCHO observations (black) and the EMAC model results (orange) for the eight regions encountered during AQABA.

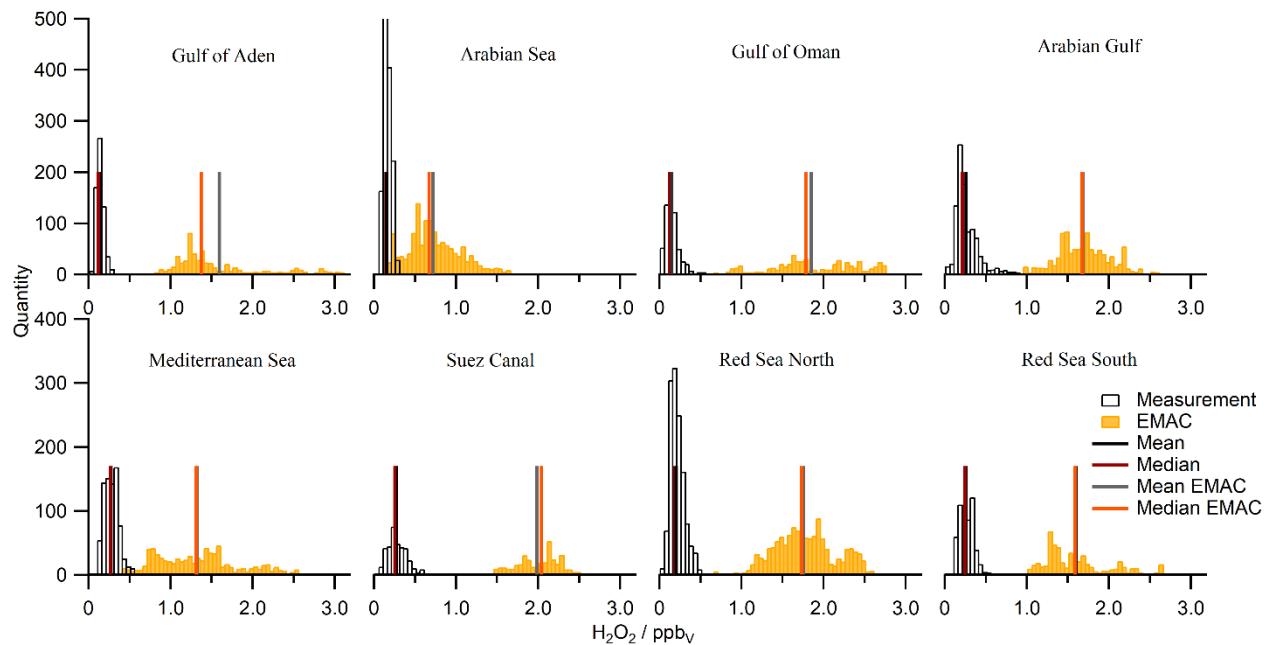


Figure S15: Frequency distributions of the H₂O₂ observations (black) and the EMAC model results (orange) for the eight regions encountered during AQABA.

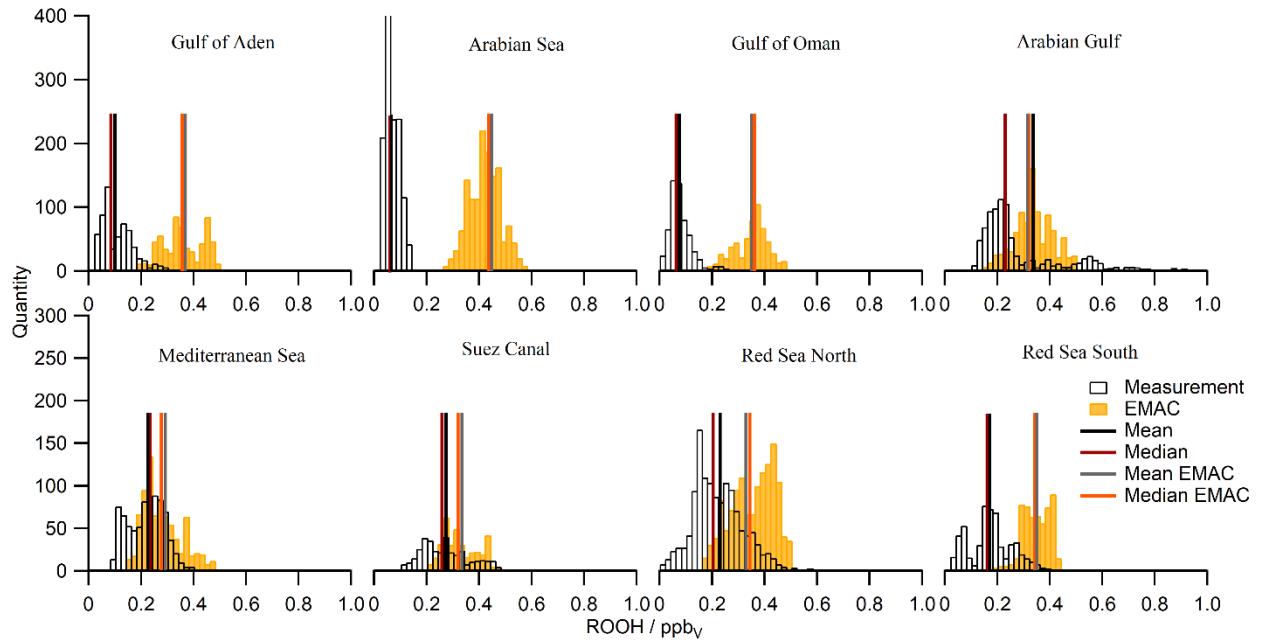


Figure S16: Frequency distributions of the ROOH observations (black) and the EMAC model results (orange) for the eight regions encountered during AQABA.

Table S2: Calculated deposition rates (k_{Dep}) of HCHO and H_2O_2 for the Arabian Sea (AS) and the Mediterranean Sea (MS). Values of k_{Dep} were determined as the slope of a linear regression (logarithmic decay versus time, Fig. 10) and the corresponding deposition velocities (V_{Dep}) are based on Eq. 12 with values for the boundary layer height derived from the ERA5 results for the corresponding timeframe ($\pm 1\sigma$). Errors of k_{Dep} and V_{Dep} are estimated to be at least $\pm 40\%$

	k_{Dep} HCHO / s^{-1}	R^2	V_{Dep} HCHO / $cm s^{-1}$	k_{Dep} H_2O_2 / s^{-1}	R^2	V_{Dep} H_2O_2 / $cm s^{-1}$	h_{BL} ERA5 / m
07. - 08.08.17	$1.75 \pm 0.70 \cdot 10^{-5}$	0.69	0.99 ± 0.40	$1.18 \pm 0.47 \cdot 10^{-5}$	0.65	0.67 ± 0.27	569 ± 12
08. - 09.08.17	$1.42 \pm 0.57 \cdot 10^{-5}$	0.47	0.66 ± 0.26	$1.91 \pm 0.76 \cdot 10^{-5}$	0.86	0.89 ± 0.36	465 ± 27
09. - 10.08.17	$0.72 \pm 0.29 \cdot 10^{-5}$	0.42	0.37 ± 0.15	$0.42 \pm 0.17 \cdot 10^{-5}$	0.70	0.22 ± 0.09	520 ± 18
10. - 11.08.17	$0.91 \pm 0.36 \cdot 10^{-5}$	0.68	0.52 ± 0.21	$1.25 \pm 0.50 \cdot 10^{-5}$	0.96	0.71 ± 0.28	573 ± 19
11. - 12.08.17	$2.18 \pm 0.87 \cdot 10^{-5}$	0.64	1.22 ± 0.49	$3.28 \pm 1.31 \cdot 10^{-5}$	0.91	1.83 ± 0.73	559 ± 18
12. - 13.08.17	$1.39 \pm 0.56 \cdot 10^{-5}$	0.59	0.82 ± 0.33	$2.72 \pm 1.09 \cdot 10^{-5}$	0.88	1.59 ± 0.64	586 ± 41
13. - 14.08.17	$1.18 \pm 0.47 \cdot 10^{-5}$	0.44	0.57 ± 0.23	$2.36 \pm 0.94 \cdot 10^{-5}$	0.82	1.14 ± 0.46	483 ± 93
14. - 15.08.17	$1.21 \pm 0.48 \cdot 10^{-5}$	0.52	0.99 ± 0.40	$1.49 \pm 0.60 \cdot 10^{-5}$	0.91	1.22 ± 0.49	822 ± 100
Mean AS ($\pm 1\sigma$)	$1.34 \pm 0.46 \cdot 10^{-5}$	0.56	0.77 ± 0.29	$1.83 \pm 0.93 \cdot 10^{-5}$	0.84	1.03 ± 0.52	572 ± 110
24. - 25.08.17	-	-	-	$0.95 \pm 0.38 \cdot 10^{-5}$	0.58	0.86 ± 0.34	906 ± 68
25. - 26.08.17	-	-	-	$2.87 \pm 1.15 \cdot 10^{-5}$	0.87	2.34 ± 0.94	814 ± 59
26. - 27.08.17	$2.20 \pm 0.88 \cdot 10^{-5}$	0.70	1.76 ± 0.70	$2.30 \pm 0.92 \cdot 10^{-5}$	0.67	1.84 ± 0.74	800 ± 63
27. - 28.08.17	$2.74 \pm 1.10 \cdot 10^{-5}$	0.56	2.22 ± 0.89	$1.68 \pm 0.67 \cdot 10^{-5}$	0.82	1.36 ± 0.54	810 ± 70
28. - 29.08.17	$2.31 \pm 0.92 \cdot 10^{-5}$	0.39	1.86 ± 0.74	$1.16 \pm 0.46 \cdot 10^{-5}$	0.54	0.94 ± 0.38	808 ± 35
29. - 30.08.17	$1.97 \pm 0.79 \cdot 10^{-5}$	0.73	1.39 ± 0.56	$1.22 \pm 0.49 \cdot 10^{-5}$	0.58	0.86 ± 0.34	706 ± 47
30. - 31.08.17	$0.33 \pm 0.13 \cdot 10^{-5}$	0.39	0.23 ± 0.09	$0.39 \pm 0.15 \cdot 10^{-5}$	0.45	0.26 ± 0.10	715 ± 68
Mean MS ($\pm 1\sigma$)	$1.91 \pm 0.93 \cdot 10^{-5}$	0.55	1.49 ± 0.76	$1.51 \pm 0.85 \cdot 10^{-5}$	0.66	1.21 ± 0.69	792 ± 74