Supplement of

Net ozone production and its relationship to nitrogen oxides and volatile organic compounds in the marine boundary layer around the Arabian Peninsula

Ivan Tadic et al.

Correspondence to: Ivan Tadic (i.tadic@mpic.de)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.
Figure S1 shows a day to day calculation of the correction factor to scale the fractional noontime integral to a diurnal value. An average ± standard deviation of (46.1 ± 2.8) % of the diurnal integral within ± 2h around noontime was estimated.

Figure S1: Ratio of the noontime actinic flux (± 2h around noon) with regard to the total actinic flux $f$(NO$_2$) of that particular day. Dashed line represents the campaign average of (46.1 ± 2.8) %. The errors bars are represented by the relative uncertainty (6 %) of the campaign average.
Figure S2: Timeline of NO, NO$_2$ (both CLD), O$_3$, OH, HO$_2$ preliminary (HO$_2^*$) and $j$(NO$_2$) data during the first leg. See Table ST2 for additional information on the ship cruise. Note that HO$_2$ data are preliminary.

Figure S3: Timeline of NO, NO$_2$ (both CLD), O$_3$, OH, HO$_2$ preliminary (HO$_2^*$) and $j$(NO$_2$) data during the second leg. See Table ST2 for additional information on the ship cruise. Note that HO$_2$ data are preliminary.
Figure S4: Ship cruises with color-scaled OH mixing ratios a) during the first and b) the second leg and color-scaled HO$_2^*$ mixing ratios c) during the first and d) the second leg. Note that OH and HO$_2^*$ data have been filtered for own stack contamination.

Figure S5: Ship cruises with color-scaled absolute humidity a) during the first and b) the second leg.
Figure S6: Scatterplot of simulated and measured regional NO$_x$ median in ppb. 1:1 line added for orientation. The error bars represent the 25-75-percentile variation.
Figure S7: Scatterplot of simulated and measured regional O$_3$ median in ppb. 1:1 line added for orientation. The error bars represent the 25-75-percentile variation.
Figure S8: Scatterplot of simulated regional (HO$_2$+RO$_2$) median and regional (HO$_2$+RO$_2$) median estimated based on measured tracer data in ppt. 1:1 line added for orientation. The error bars represent the 25-75-percentile variation.
Figure S9: Scatterplot of median NOPR in ppb, day\(^{-1}\) estimated based on simulated and measured tracer data. 1:1 line added for orientation. The error bars represent the 25-75-percentile variation.
Figure S10: Comparison of the regional, absolute contribution of $k_{\text{NO}+\text{HO}_2}[\text{NO}]/([\text{HO}_2] + [\text{RO}_2])$ to NOPR in the six different regions investigated during AQABA. The horizontal black bar indicates the median value, the box the 25- and 75-percentiles and the whiskers the 10- and 90-percentiles.
Figure S11: Comparison of the regional, absolute contribution of $-j(O^1D) \cdot \alpha \cdot [O_3]$ to NOPR in the six different regions investigated during AQABA. The horizontal black bar indicates the median value, the box the 25- and 75-percentiles and the whiskers the 10- and 90-percentiles.
Figure S12: Comparison of the regional, absolute contribution of $-k_{\text{HO}_2+O_3}[\text{HO}_2][O_3]$ to NOPR in the six different regions investigated during AQABA. The horizontal black bar indicates the median value, the box the 25- and 75-percentiles and the whiskers the 10- and 90-percentiles.
Figure S13: Comparison of the regional, absolute contribution of $-k_{\text{OH}+O_3}[\text{OH}][O_3]$ to NOPR in the six different regions investigated during AQABA. The horizontal black bar indicates the median value, the box the 25- and 75-percentiles and the whiskers the 10- and 90-percentiles.
Table ST1: Range of latitudinal and longitudinal coordinates and dates during both legs of the different regions.

| region (abbreviation) | latitudinal range      | longitudinal range      | Date (1\textsuperscript{st} leg) | Date (2\textsuperscript{nd} leg) |
|-----------------------|------------------------|-------------------------|----------------------------------|----------------------------------|
| Mediterranean (M)     | 31.810° N- 39.923° N   | 12.620° E- 31.850° E    | ---                              | 25.08.2017 – 31.08.2017          |
| Northern Red Sea (NRS)| 23.343° N- 30.986° N   | 32.305° E- 37.085° E    | 03.07.2017 – 08.07.2017          | 21.08.2017 – 24.08.2017          |
| Southern Red Sea (SRS)| 12.672° N- 22.494° N   | 37.411° E- 43.327° E    | 09.07.2017 – 16.07.2017          | 17.08.2017 – 20.08.2017          |
| Arabian Sea (AS)      | 11.797° N- 22.782° N   | 44.035° E- 60.636° E    | 18.07.2017 – 24.07.2017          | 07.08.2017 – 16.08.2017          |
| Oman Gulf (OG)        | 23.050° N- 25.622° N   | 56.492° E- 59.913° E    | 24.07.2017 – 27.07.2017          | 05.08.2017 – 07.08.2017          |
| Arabian Gulf (AG)     | 25.396° N- 29.425° N   | 47.920° E- 56.772° E    | 27.07.2017 – 31.07.2017          | 03.08.2017 – 05.08.2017          |
Table ST2: Overview of the time spent in the particular regions during AQABA. Red color indicates periods with KI at anchor that are not included in the data analysis. Data measured during bunkering at Fujairah City (06 August, 07:00-15:00 UTC) were also not included in the analysis.

| Date       | Region                      | Date       | Region                          |
|------------|------------------------------|------------|---------------------------------|
| 03.07.2017 | Northern Red Sea            | 02.08.2017 | Kuwait port                     |
| 04.07.2017 | Northern Red Sea            | 03.08.2017 | Kuwait port/Arabian Gulf        |
| 05.07.2017 | Northern Red Sea            | 04.08.2017 | Arabian Gulf                    |
| 06.07.2017 | Northern Red Sea            | 05.08.2017 | Arabian Gulf/Oman Gulf          |
| 07.07.2017 | Northern Red Sea            | 06.08.2017 | Oman Gulf                       |
| 08.07.2017 | Northern Red Sea            | 07.08.2017 | Oman Gulf/Arabian Sea           |
| 09.07.2017 | Southern Red Sea            | 08.08.2017 | Arabian Sea                     |
| 10.07.2017 | Southern Red Sea            | 09.08.2017 | Arabian Sea                     |
| 11.07.2017 | Southern Red Sea/Jeddah port| 10.08.2017 | Arabian Sea                     |
| 12.07.2017 | Jeddah port                 | 11.08.2017 | Arabian Sea                     |
| 13.07.2017 | Jeddah port/Southern Red Sea| 12.08.2017 | Arabian Sea                     |
| 14.07.2017 | Southern Red Sea            | 13.08.2017 | Arabian Sea                     |
| 15.07.2017 | Southern Red Sea            | 14.08.2017 | Arabian Sea                     |
| 16.07.2017 | Southern Red Sea            | 15.08.2017 | Arabian Sea                     |
| 17.07.2017 | Djibouti port               | 16.08.2017 | Arabian Sea                     |
| 18.07.2017 | Arabian Sea                 | 17.08.2017 | Southern Red Sea                |
| 19.07.2017 | Arabian Sea                 | 18.08.2017 | Southern Red Sea                |
| 20.07.2017 | Arabian Sea                 | 19.08.2017 | Southern Red Sea                |
| 21.07.2017 | Arabian Sea                 | 20.08.2017 | Southern Red Sea                |
| 22.07.2017 | Arabian Sea                 | 21.08.2017 | Northern Red Sea                |
| 23.07.2017 | Arabian Sea                 | 22.08.2017 | Northern Red Sea                |
| 24.07.2017 | Arabian Sea/Oman Gulf       | 23.08.2017 | Northern Red Sea                |
| 25.07.2017 | Oman Gulf                   | 24.08.2017 | Northern Red Sea                |
| 26.07.2017 | Oman Gulf                   | 25.08.2017 | Mediterranean                   |
| 27.07.2017 | Oman Gulf/Arabian Gulf      | 26.08.2017 | Mediterranean                   |
| 28.07.2017 | Arabian Gulf                | 27.08.2017 | Mediterranean                   |
| 29.07.2017 | Arabian Gulf                | 28.08.2017 | Mediterranean                   |
| 30.07.2017 | Arabian Gulf                | 29.08.2017 | Mediterranean                   |
| 31.07.2017 | Arabian Gulf/Kuwait port     | 30.08.2017 | Mediterranean                   |
| 01.08.2017 | Kuwait port                 | 31.08.2017 | Mediterranean                   |
Table ST3: Overview of measured NO\textsubscript{x} (upper table) and measured O\textsubscript{3} (lower table) spatial volume mixing ratio average, standard deviation, 1\textsuperscript{st} quantile, median, 3\textsuperscript{rd} quantile (all in ppb\textsubscript{v}) and number of considered data points.

| NO\textsubscript{x} (upper), O\textsubscript{3} (lower) | Mediterranea n | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|-----------------------------------------------------|----------------|------------------|------------------|-------------|-----------|-------------|
| data points                                        | 1767           | 1694             | 1755             | 2656        | 1056      | 1539        |
| average                                            | 1.24           | 4.69             | 1.62             | 0.95        | 4.16      | 3.65        |
| stdev                                              | 3.34           | 7.9              | 3.7              | 3.15        | 4.33      | 9.24        |
| 1\textsuperscript{st} quantile                    | 0.12           | 0.68             | 0.18             | 0.10        | 1.03      | 0.52        |
| median                                             | 0.25           | 1.76             | 0.46             | 0.19        | 2.74      | 1.26        |
| 3\textsuperscript{rd} quantile                    | 0.96           | 5.68             | 1.6              | 0.54        | 5.92      | 3.47        |

| data points                                        | 2010           | 2717             | 2307             | 4130        | 1249      | 1809        |
| average                                            | 61.56          | 63.39            | 50.35            | 21.53       | 34.04     | 73.99       |
| stdev                                              | 8.25           | 18.45            | 12.96            | 6.8         | 11.27     | 35.68       |
| 1\textsuperscript{st} quantile                    | 57.05          | 53.51            | 40.68            | 17.45       | 26.66     | 53.08       |
| median                                             | 61.54          | 64.16            | 46.93            | 22.52       | 31.5      | 62.5        |
| 3\textsuperscript{rd} quantile                    | 66.48          | 75.51            | 60.28            | 26.19       | 38.03     | 90.42       |

Table ST4: Overview of simulated NO\textsubscript{x} (upper table) and simulated O\textsubscript{3} (lower table) spatial volume mixing ratio average, standard deviation, 1\textsuperscript{st} quantile, median, 3\textsuperscript{rd} quantile (all in ppb\textsubscript{v}) and number of considered data points.

| NO\textsubscript{x} (upper), O\textsubscript{3} (lower) | Mediterranea n | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|-----------------------------------------------------|----------------|------------------|------------------|-------------|-----------|-------------|
| data points                                        | 2012           | 2719             | 2310             | 4464        | 1253      | 1810        |
| average                                            | 0.84           | 1.27             | 1.13             | 0.31        | 1.88      | 1.91        |
| stdev                                              | 0.75           | 1.97             | 0.62             | 0.29        | 1.47      | 1.37        |
| 1\textsuperscript{st} quantile                    | 0.33           | 0.43             | 0.67             | 0.14        | 0.82      | 1.17        |
| median                                             | 0.43           | 0.76             | 0.97             | 0.18        | 1.59      | 1.61        |
| 3\textsuperscript{rd} quantile                    | 1.27           | 1.08             | 1.51             | 0.39        | 2.05      | 2.16        |

| data points                                        | 2012           | 2719             | 2310             | 4464        | 1253      | 1810        |
| average                                            | 65.15          | 64.76            | 49.5             | 36.91       | 55        | 76.85       |
| stdev                                              | 4.99           | 7.7              | 7.21             | 3.87        | 9.94      | 12.8        |
| 1\textsuperscript{st} quantile                    | 61.35          | 60.34            | 43.47            | 34.12       | 48.37     | 65.88       |
| median                                             | 65.53          | 64.6             | 49.33            | 36.54       | 55.01     | 76.39       |
| 3\textsuperscript{rd} quantile                    | 69.33          | 68.25            | 54.58            | 38.85       | 61.42     | 86.22       |
Table ST5: Overview of noontime (HO$_2$+RO$_2$) spatial volume mixing ratio average, standard deviation, 1$^{st}$ quantile, median, 3$^{rd}$ quantile (all in ppt) estimated based on measured tracer data. Number of considered data points added in the first line.

| HO$_2$+RO$_2$ | Mediterranean | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|---------------|--------------|------------------|------------------|-------------|-----------|-------------|
| data points   | 288          | 126              | 190              | 338         | 166       | 242         |
| average       | 13           | 27               | 7                | 64          | 23        | 94          |
| stdev         | 24           | 20               | 34               | 83          | 42        | 113         |
| 1$^{st}$ quantile | 1       | 15               | -13              | 23          | -8        | 11          |
| median        | 16           | 28               | 15               | 33          | 22        | 73          |
| 3$^{rd}$ quantile | 26      | 44               | 27               | 54          | 49        | 176         |

Table ST6: Overview of simulated noontime (HO$_2$+RO$_2$) spatial volume mixing ratio average, standard deviation, 1$^{st}$ quantile, median, 3$^{rd}$ quantile (all in ppt). Number of considered data points added in the first line.

| HO$_2$+RO$_2$ | Mediterranean | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|---------------|--------------|------------------|------------------|-------------|-----------|-------------|
| data points   | 336          | 192              | 192              | 720         | 203       | 293         |
| average       | 41           | 46               | 36               | 40          | 48        | 49          |
| stdev         | 5            | 4                | 11               | 5           | 6         | 7           |
| 1$^{st}$ quantile | 36      | 43               | 25               | 38          | 44        | 44          |
| median        | 41           | 46               | 38               | 41          | 50        | 49          |
| 3$^{rd}$ quantile | 46      | 49               | 42               | 43          | 53        | 54          |

Table ST7: Overview of NOPR average, standard deviation, 1$^{st}$ quantile, median, 3$^{rd}$ quantile (all in ppb, day$^{-1}$) estimated based on measured tracer data. Number of considered data points added in the first line.

| NOPR | Mediterranean | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|------|--------------|------------------|------------------|-------------|-----------|-------------|
| data points | 148          | 114              | 89               | 187         | 84        | 111         |
| average     | -3           | 16               | -5               | -67         | -105      | -24         |
| stdev       | 43           | 39               | 12               | 576         | 362       | 449         |
| 1$^{st}$ quantile | -5     | 6                | -9               | 1           | -18       | 25          |
| median      | -1           | 16               | -4               | 5           | 16        | 32          |
| 3$^{rd}$ quantile | 8      | 40               | -1               | 11          | 23        | 65          |
Table ST8: Overview of NOPR average, standard deviation, 1st quantile, median, 3rd quantile (all in ppb·day⁻¹) estimated based on simulated tracer data. Number of considered data points added in the first line.

| NOPR          | Mediterranean | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|---------------|---------------|------------------|------------------|-------------|-----------|--------------|
| data points   | 336           | 192              | 192              | 720         | 203       | 293          |
| average       | 11            | 16               | 12               | 5           | 30        | 38           |
| stddev        | 8             | 12               | 6                | 6           | 11        | 10           |
| 1st quantile | 5             | 8                | 8                | 1           | 22        | 30           |
| median        | 8             | 12               | 11               | 2           | 28        | 35           |
| 3rd quantile | 17            | 21               | 15               | 10          | 37        | 46           |

Table ST9: Overview of measured HCHO/NO₂-ratio average, standard deviation, 1st quantile, median, 3rd quantile and number of considered data points.

| Ratio          | Mediterranean | Northern Red Sea | Southern Red Sea | Arabian Sea | Oman Gulf | Arabian Gulf |
|----------------|---------------|------------------|------------------|-------------|-----------|--------------|
| data points    | 203           | 79               | 48               | 252         | 108       | 122          |
| average        | 5.4           | 1.5              | 8.5              | 11.1        | 2.7       | 9            |
| stddev         | 4.7           | 0.7              | 6.5              | 8.9         | 2.1       | 6.4          |
| 1st quantile  | 1.3           | 0.8              | 4.4              | 2.3         | 1         | 2.5          |
| median         | 5             | 1.4              | 7.7              | 9.4         | 2.2       | 9.3          |
| 3rd quantile  | 7.4           | 2.1              | 9.8              | 16.1        | 3.6       | 12.7         |
Table ST10: List of included peroxy radicals (with less than four carbon atoms) for the reaction with NO as recommended by Sander et al. (2019).

| Species                                                                 |
|------------------------------------------------------------------------|
| HO₂                                                                     |
| CH₃O₂                                                                  |
| C₂H₅O₂                                                                 |
| C₂H₅CO₃                                                                |
| CH₃CO₃                                                                 |
| C₃DIALO₂ (C₃H₃O₄)                                                     |
| CH₃CHOHO₂                                                              |
| CH₃COCH₂O₂                                                             |
| CH₃COCO₃                                                               |
| CHOCHOCH₂O₂                                                            |
| CO₂H₃CO₃                                                               |
| HCOCH₂CO₃                                                             |
| HCOCH₂O₂                                                               |
| HCOCO₃                                                                |
| HCOCOCHCO₃                                                            |
| HOC₂H₄CO₃                                                             |
| HOCH₂CH₂O₂                                                             |
| HOCH₂CO₃                                                               |
| HOCH₂COCH₂O₂                                                           |
| HOCH₂O₂                                                                |
| CH₃CHO₂CH₂OH                                                           |
| IC₃H₇O₂ (isopropylperoxy radical)                                     |
| NC₃H₇O₂ (propylperoxy radical)                                        |
| NCCH₂O₂                                                                |
| NO₃CH₂CO₃                                                              |
| CH₃CHO₂CH₂ONO₂                                                         |