# Supplemental material

# Evaluation of simulated $O_3$ production efficiency during the KORUS-AQ campaign: Implications for anthropogenic $NO_x$ emissions in Korea

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**Figure S1. Comparison of observed and simulated $NO_2$ and radical species**

Box-plot comparison of observed and simulated $NO_2$, OH, $HO_2$, and $RO_2$ (total organic peroxy radicals, no observations available) below 1.5 km during 13-16 LST. The bars and lines each indicate the interquartile range and the 10-90th percentiles, respectively, and the diamond indicates the median value.

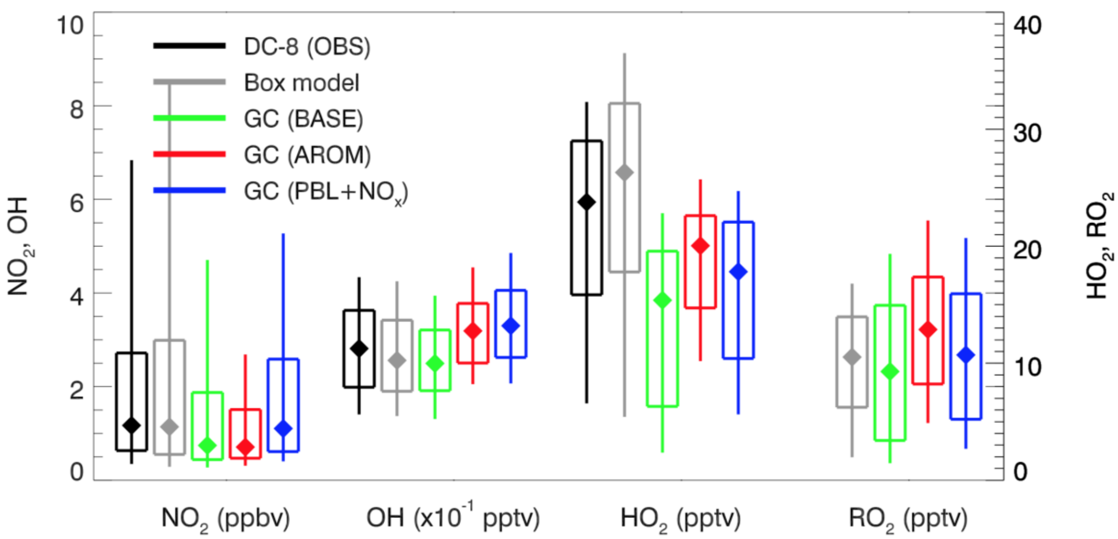

**Figure S2. Comparison of observed and simulated organic nitrates, PAN, and speciated VOCs**

Box-plot comparison of observed and simulated organic nitrates, PAN, and VOCs below 1.5 km during 13-16 LST. The bars and lines each indicate the interquartile range and the 10-90th percentiles, respectively, and the diamond indicates the median value. For comparison of >C4 alkanes and >C3 alkenes, total amounts of measured alkane species with four or more carbons and alkene species with three or more carbons were considered.

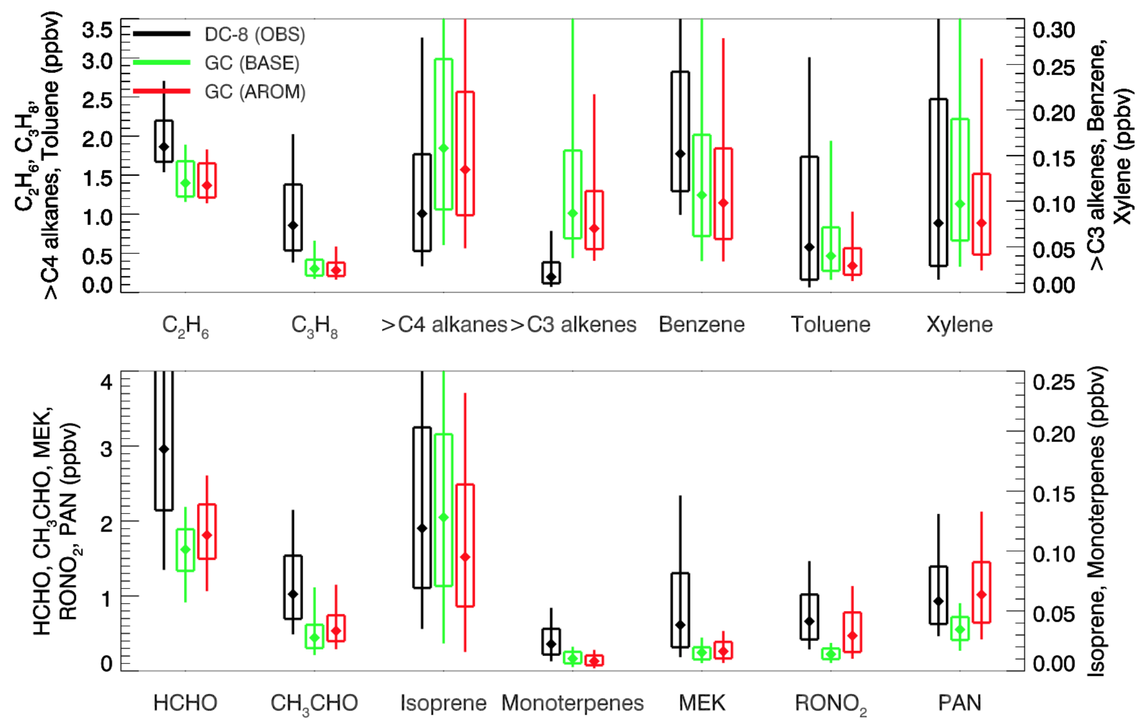

**Figure S3. Mean sea level pressures (SLP) and wind vectors in GEOS-Chem during four different synoptic weather patterns in East Asia**

Mean sea level pressures (colors and contours) and wind vectors (blue arrows) in the GEOS-FP assimilated meteorological field used in GEOS-Chem. Each figure indicates periods with different synoptic weather patterns; a) dynamic weather period, b) stagnant period, c) extreme pollution period, and d) blocking pattern period.

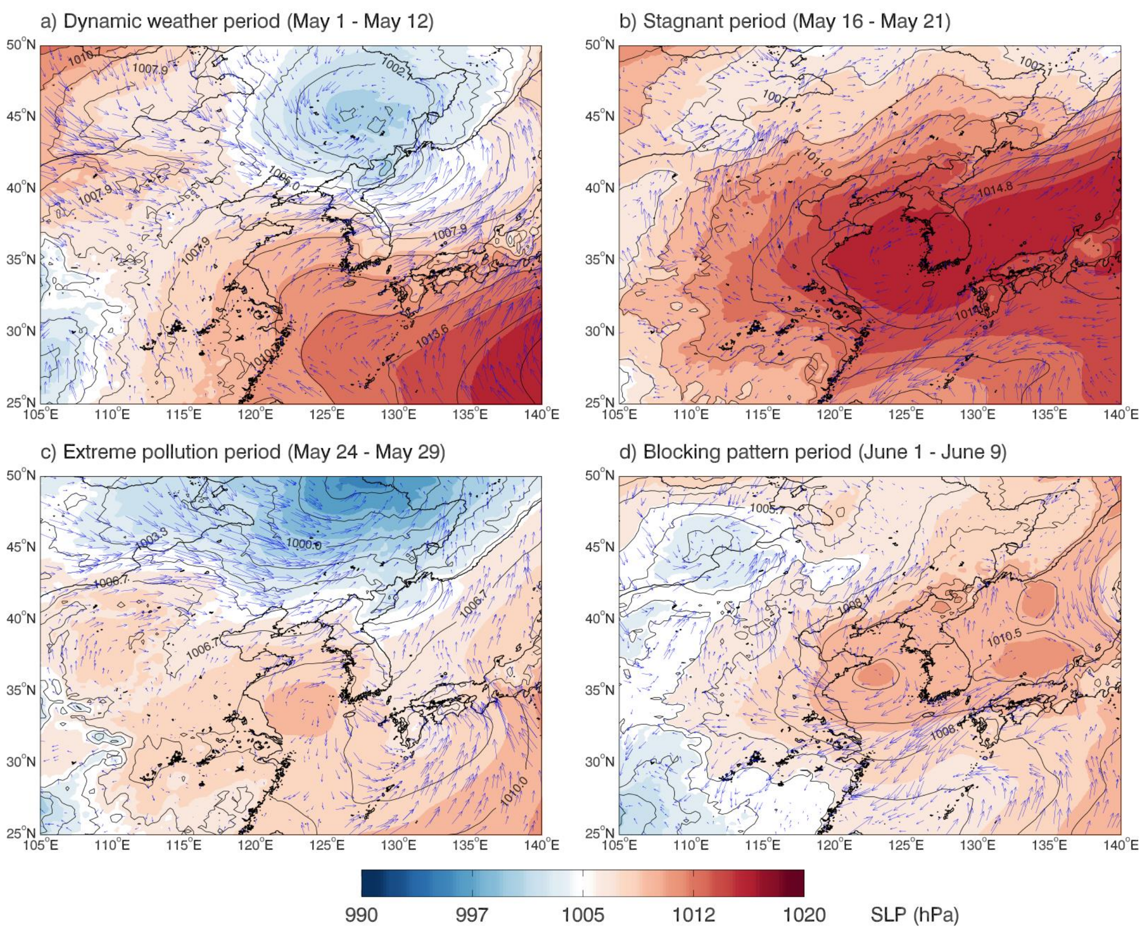

**Table S1. Gas phase reactions of aromatic chemistry in GEOS-Chem based on Henze et al. (2008)**

| Reactants | Products | Rate constant [a] | | |
|---|---|---|---|---|
| **Kinetic reactions** | | A | B | C |
| BENZ + OH | 1.000BRO2 | 2.33E-12 | 0 | -193 |
| TOLU + OH | 1.000TRO2 | 1.81E-12 | 0 | 338 |
| XYLE + OH | 1.000XRO2 | 2.31E-11 | 0 | 0 |
| BRO2 + HO2 | 1.000LBRO2H | 1.40E-12 | 0 | 700 |
| BRO2 + NO | 1.000LBRO2N | 2.60E-12 | 0 | 350 |
| TRO2 + HO2 | 1.000LTRO2H | 1.40E-12 | 0 | 700 |
| TRO2 + NO | 1.000LTRO2N | 2.60E-12 | 0 | 350 |
| XRO2 + HO2 | 1.000LXRO2H | 1.40E-12 | 0 | 700 |
| XRO2 + NO | 1.000LXRO2N | 2.60E-12 | 0 | 350 |

[b] Rate constants for kinetic reactions are calculated following the Arrhenius equation form of $k = A\left(\frac{300}{T}\right)^{B} exp\left(\frac{C}{T}\right)$, where T indicates temperature.

**Table S2. Gas phase reactions of aromatic chemistry added in GEOS-Chem based on Porter et al. (2017)**

| Reactants | Products | Rate constant [a] | | |
|---|---|---|---|---|
| **Kinetic reactions** | | A | B | C |
| BENZ + OH | 0.352BRO2 + 0.530PHEN + 0.648HO2 + 0.120EPX | 2.33E-12 | 0 | -193 |
| TOLU + OH | 0.750TRO2 + 0.250CRES + 0.250HO2 | 1.81E-12 | 0 | 354 |
| XYLE + OH | 0.830XRO2 + 0.170CRES + 0.170HO2 | 2.31E-11 | 0 | 0 |
| BRO2 + HO2 | 1.000LBRO2H + 3.000ETP | 2.24E-13 | 0 | 1300 |
| BRO2 + NO | 0.920NO2 + 0.920HO2 + 0.920GLYX + 0.840DCB + 1.000LBRO2N | 2.54E-12 | 0 | 360 |
| BRO2 + MO2 | 1.000CH2O + 0.160HO2 + 0.960DCB + 0.600GLYX | 3.56E-14 | 0 | 708 |
| BRO2 + MCO3 | 1.000MO2 + 0.600HO2 + 0.600GLYX + 1.160DCB | 7.40E-13 | 0 | 765 |
| BRO2 + NO3 | 1.000NO2 + 1.000HO2 + 1.000GLYX + 0.800DCB | 1.20E-12 | 0 | 0 |
| TRO2 + HO2 | 1.000LTRO2H + 3.500ETP | 2.39E-13 | 0 | 1300 |
| TRO2 + NO | 1.000NO2 + 1.000HO2 + 0.160GLYX + 0.170MGLY + 0.700DCB + 1.000LTRO2N | 4.20E-12 | 0 | 180 |
| TRO2 + MO2 | 1.000CH2O + 2.000HO2 + 0.700DCB + 0.160GLYX + 0.170MGLY | 1.70E-14 | 0 | 220 |
| TRO2 + MCO3 | 1.000MO2 + 1.000HO2 + 0.160GLYX + 0.170MGLY + 0.700DCB | 4.20E-14 | 0 | 220 |
| XRO2 + HO2 | 1.000LXRO2H + 4.000ETP | 2.50E-13 | 0 | 1300 |
| XRO2 + NO | 1.000NO2 + 1.000HO2 + 0.806DCB + 0.450MGLY + 1.000LXRO2N | 4.20E-12 | 0 | 180 |
| XRO2 + MO2 | 1.000CH2O + 2.000HO2 + 0.860DCB + 0.450MGLY | 1.70E-14 | 0 | 220 |
| XRO2 + MCO3 | 1.000MO2 + 1.000HO2 + 0.806DCB + 0.450MGLY | 4.20E-14 | 0 | 220 |
| PHEN + OH | 0.900XO2 + 0.100HO2 + 0.900MCO3 | 6.75E-12 | 0 | 405 |
| PHEN + NO3 | 1.000XNO2 + 1.000HNO3 + 0.500CRES | 3.78E-12 | 0 | 0 |

| | | | | |
|---|---|---|---|---|
| CRES + OH | 0.900XO2 + 0.100HO2 + 0.900MCO3 | 4.00E-12 | 0 | 0 |
| CRES + NO3 | 1.000HNO3 + 1.000XNO2 + 0.500CRES | 2.20E-11 | 0 | 0 |
| EPX + OH | 1.000XO2 + 1.000HO2 + 1.000CO + 1.000RCHO | 2.80E-12 | 0 | 275 |
| EPX + NO3 | 1.000GLYX + 1.500HO2 + 0.500NO2 + 0.500HNO3 + 0.500CO2 + 1.500CO + 0.500OH | 2.87E-13 | 0 | -1000 |
| TCO3 + NO | 1.000NO2 + 0.920HO2 + 0.890GLYX + 0.050MCO3 + 0.110MGLY | 4.20E-11 | 0 | 180 |
| TCO3 + MO2 | 0.500CH2O + 0.500ACTA + 0.460HO2 + 0.475CO + 0.055MGLY + 0.025MCO3 + 0.445GLYX + 1.000XO2 | 9.60E-13 | 0 | 220 |
| TCO3 + MCO3 | 1.000MO2 + 0.920HO2 + 0.890GLYX + 0.110MGLY + 0.050MCO3 + 0.950CO + 2.000XO2 | 1.19E-12 | 0 | 220 |
| TCO3 + HO2 | 1.000ETP | 7.70E-14 | 0 | 1300 |
| XO2 + HO2 | 1.000ETP | 7.70E-14 | 0 | 1300 |
| XO2 + MO2 | 1.000CH2O + 1.000HO2 | 1.70E-14 | 0 | 220 |
| XO2 + MCO3 | 1.000MO2 | 4.20E-14 | 0 | 220 |
| XO2 + NO | 1.000NO2 | 4.20E-12 | 0 | 180 |
| XNO2 + NO2 | 1.000R4N2 | 4.20E-12 | 0 | 180 |
| XNO2 + HO2 | 1.000ETP | 7.70E-14 | 0 | 1300 |
| XNO2 + MO2 | 1.000CH2O + 1.000HO2 | 1.70E-14 | 0 | 220 |
| XNO2 + MCO3 | 1.000MO2 | 4.20E-14 | 0 | 220 |
| DCB + OH | 1.000MCO3 + 1.000HO2 | 2.80E-11 | 0 | 0 |
| DCB + NO3 | 1.000HNO3 + 1.000TCO3 | 1.40E-12 | 0 | -1900 |
| **Photolysis reactions** | | | | |
| DCB | 0.980HO2 + 1.000TCO3 + 0.020MCO3 | $J(NO_2)$ * 0.14 | | |

[b] Rate constants for kinetic reactions are calculated following the Arrhenius equation form of $k = A\left(\frac{300}{T}\right)^{B} exp\left(\frac{C}{T}\right)$, where T indicates temperature.

**Table S3. Aromatic species and reaction intermediates added in GEOS-Chem**

| Species name | Description |
|---|---|
| CRES | Cresol |
| PHEN | Phenol |
| EPX | Epoxide from BENZ |
| DCB | Unsaturated dicarbonyls |
| TCO3 | Unsaturated acyl peroxy radical |
| XO2 | RO2 from CRES, PHEN, EPX |
| XNO2 | RO2 containing nitro groups from CRES, PHEN |