Supplement of

Multiphase MCM–CAPRAM modeling of the formation and processing of secondary aerosol constituents observed during the Mt. Tai summer campaign in 2014

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Table S1. Emission data applied in the SPACCIM (*: anthropogenic emission values, #: biogenic emission values).

| Compound                  | Emission / molec cm\(^{-3}\) s\(^{-1}\) | Compound                  | Emission / molec cm\(^{-3}\) s\(^{-1}\) |
|---------------------------|------------------------------------------|---------------------------|------------------------------------------|
| Acetone*                  | 3.51E+04                                 | Acetaldehyde*             | 1.44E+04                                 |
| Ethane*                   | 1.30E+05                                 | Ethylene*                 | 1.76E+05                                 |
| Propane*                  | 1.87E+05                                 | Glyoxal*                  | 1.04E+04                                 |
| n-Butane*                 | 6.79E+04                                 | Formaldehyde*             | 3.15E+04                                 |
| Isobutane*                | 2.99E+04                                 | Biacetyl*                 | 1.49E+03                                 |
| 2,2-Dimethyl Butane*      | 2.00E+03                                 | Benzaldehyde*             | 3.37E+02                                 |
| Isopentane*               | 6.75E+04                                 | Methacrolein*             | 2.08E+03                                 |
| n-Pentane*                | 2.67E+04                                 | Methyl ethyl ketone*      | 8.68E+03                                 |
| 2-Methyl Pentane*         | 1.57E+04                                 | Methanol*                 | 2.28E+04                                 |
| 3-Methylpentane*          | 1.10E+04                                 | Methylglyoxal*            | 3.93E+03                                 |
| n-Hexane*                 | 6.28E+03                                 | Methyl Vinyl Ketone*      | 2.62E+02                                 |
| n-Heptane*                | 4.71E+03                                 | Propene*                  | 2.96E+04                                 |
| 2,3-Dimethyl Butane*      | 4.71E+03                                 | 1-Hexene*                 | 2.45E+04                                 |
| n-Decane*                 | 1.77E+04                                 | 1-Butene*                 | 1.22E+04                                 |
| 3-Methyl Hexane*          | 1.77E+04                                 | 1-Pentene*                | 1.12E+04                                 |
| n-Nonane*                 | 6.45E+03                                 | 3-Methyl-1-Butene*        | 3.06E+03                                 |
| n-Octane*                 | 6.45E+03                                 | cis-2-Pentene*            | 2.25E+04                                 |
| 2-Methyl Hexane*          | 4.84E+03                                 | trans-2-Pentene*          | 2.25E+04                                 |
| n-Dodecane*               | 3.22E+03                                 | 1,3-Butadiene*            | 9.64E+03                                 |
| n-Undecane*               | 1.61E+03                                 | 2-Methyl-2-Butene*        | 8.03E+03                                 |
| Toluene*                  | 1.39E+05                                 | Cis-2-Hexene*             | 8.03E+03                                 |
| Ethyl Benzene*            | 1.86E+04                                 | Trans-2-Hexene*           | 8.03E+03                                 |
| n-Propyl Benzene*         | 7.43E+03                                 | Propionaldehyde*          | 6.40E+03                                 |
| Isopropyl Benzene*        | 3.72E+03                                 | Limonene*                 | 3.28E+02                                 |
| m-Xylene*                 | 1.46E+04                                 | Carbon monoxide*          | 3.04E+07                                 |
| p-Xylene*                 | 1.46E+04                                 | Carbon dioxide*           | 1.15E+09                                 |
| o-Xylene*                 | 1.23E+04                                 | Ammonia*                  | 3.81E+06                                 |
| 1,2,3-Trimethyl Benzene*  | 1.01E+04                                 | Nitric Oxide*             | 2.51E+05                                 |
| 1,3,5-Trimethyl Benzene*  | 1.01E+04                                 | Nitrogen dioxide*         | 1.42E+06                                 |
### Table S2. Deposition velocities applied in the SPACCIM.

| Compound                      | Deposition / s\(^{-1}\) | Compound                      | Deposition / s\(^{-1}\) |
|-------------------------------|--------------------------|-------------------------------|--------------------------|
| Methanol                      | 1.00E-05                 | N\(_2\)O\(_5\)               | 2.00E-05                 |
| Carbon monoxide               | 1.00E-06                 | Ammonia                      | 1.00E-05                 |
| Ethanol                       | 5.00E-06                 | Nitrogen dioxide             | 4.00E-06                 |
| Hydrogen peroxide             | 1.00E-05                 | Ozone                        | 4.00E-06                 |
| Formaldehyde                  | 1.00E-05                 | Formic acid                  | 1.00E-05                 |
| Hydrochloric acid             | 1.00E-05                 | Sulfur dioxide               | 1.00E-05                 |
| Nitric acid                   | 2.00E-05                 | Sulfuric acid                | 2.00E-05                 |

### Table S3. Initial gas-phase concentrations applied in the SPACCIM.

| Compound                    | Concentration | Compound                    | Concentration |
|-----------------------------|---------------|-----------------------------|---------------|
| Nitric oxide                | 0.32 ppbv     | p-Xylene                    | 94.53 pptv    |
| Nitrogen dioxide            | 1.72 ppbv     | m-Xylene                    | 94.53 pptv    |
| Ozone                       | 100.33 ppbv   | Acetaldehyde                | 1.00 ppbv     |
| Nitric acid                 | 0.67 ppbv     | Propionaldehyde             | 70.48 pptv    |
| Hydrogen peroxide           | 0.31 ppbv     | Butyraldehyde               | 35.32 pptv    |
| Formaldehyde                | 0.70 ppbv     | Acetone                     | 1.07 ppbv     |
| Hydrogen                    | 0.46 ppmv     | Methyl ethyl ketone         | 29.44 pptv    |
| Carbon monoxide             | 1.18 ppmv     | Methyl isobutyl ketone      | 13.02 pptv    |
| Methane                     | 2.06 ppmv     | Glyoxal                     | 0.21 ppbv     |
| Carbon dioxide              | 332.10 ppmv   | Glycolaldehyde              | 0.21 ppbv     |
| Sulfur dioxide              | 2.14 ppbv     | Methylglyoxal               | 18.57 pptv    |
| Ethane                      | 0.43 ppbv     | Peroxyacetyl nitrate        | 92.87 pptv    |
| Propane                     | 80.43 pptv    | Methyl hydrogen peroxide    | 0.19 ppbv     |
| Compound               | Data / $g_{\text{compound}} g_{\text{aerosol}}^{-1}$ | Parameter               | Data               |
|------------------------|-----------------------------------------------------|-------------------------|--------------------|
| Isoprene               | 96.19 pptv                                          | Ethyl hydrogen peroxide | 18.57 pptv         |
| n-propanol             | 1.30 pptv                                          | Peroxyacetic acid       | 0.19 pptv          |
| Isopropanol            | 51.00 pptv                                          | Ammonia                 | 4.39 ppbv          |
| Butanol                | 0.75 pptv                                          | Methanol                | 0.42 ppbv          |
| Isobutanol             | 0.56 pptv                                          | Ethanol                 | 0.40 ppbv          |
| Ethylene glycol        | 1.17 pptv                                          | Glyoxylic acid          | 0.11 ppbv          |
| Ethylene               | 0.96 ppbv                                          | Glycolic acid           | 0.11 ppbv          |
| Toluene                | 0.31 ppbv                                          |                         |                    |
| Cresol                 | 0.19 pptv                                          |                         |                    |
| o-Xylene               | 62.61 pptv                                          |                         |                    |

**Table S4. Aerosol compositions and parameters applied in the SPACCIM.**

| Compound                        | Data / $g_{\text{compound}} g_{\text{aerosol}}^{-1}$ | Parameter                     | Data               |
|---------------------------------|-----------------------------------------------------|-------------------------------|--------------------|
| Sulfate                         | 0.25                                                | Aerosol radius                | 2.0E-07 m          |
| Nitrate                         | 0.21                                                | Aerosol Density               | 1770 kg m$^{-3}$   |
| Ammonium                        | 0.16                                                | Aerosol number concentration  | 5.1E+08 m$^{-3}$   |
| Water-soluble organic carbon    | 0.07                                                |                               |                    |
| HULIS                           | 0.07                                                |                               |                    |
| Water-insoluble organic carbon  | 0.05                                                |                               |                    |
| Positive monovalent ions        | 0.03                                                |                               |                    |
| Positive divalent ions          | 0.01                                                |                               |                    |
| Metals                          | 0.03                                                |                               |                    |
| Elemental carbon                | 0.03                                                |                               |                    |
Figure S1. Three-day back-trajectories for Mt. Tai during the sampling period (green triangle: Mt. Tai).
Figure S2. Meteorological data in different scenarios.
Figure S3. Time series of the modeled radical oxidant concentrations in the C4w and C4wo cases (light blue column: cloud; shadow: night).
Figure S4. Time series of the modeled non-radical oxidant concentrations in the C4w and C4wo cases (light blue column: cloud; shadow: night; green triangle: maximum (above), average (middle) and minimum (below) value of measured concentration at Mt. Tai).

Figure S5. Time series of the modeled concentrations of key secondary inorganic ions in the C4w and C4wo cases (light blue column: cloud; shadow: night; green triangle: maximum (above), average (middle) and minimum (below) value of measured concentrations at Mt. Tai).
Figure S6. Modeled source and sink fluxes of sulfate (left) and nitrate (right) in the C2wo case (shadow: night).

Figure S7. Scatter plot of the concentrations between Pyr and H₂O₂ in the C2wo case.
Figure S8. Time series of the modeled concentrations of selected DCRCs in the C4w and C4wo cases (light blue column: cloud; shadow: night; green triangle: maximum (above), average (middle) and minimum (below) value of measured concentration at Mt. Tai).
Figure S9. Modeled source and sink fluxes of glyoxylic (above left), oxalic (above right), pyruvic (below left) and malonic (below right) acid in the C2wo case (shadow: night).
Figure S10. Key oxidants for the source compounds of oxalic (above) and glyoxylic (below) acid in the C2w (left) and C2wo (right) cases.