## Supplementary Material for the ACP manuscript "Predicting Secondary Organic Aerosol Phase State and Viscosity and its Effect on Multiphase Chemistry in a Regional Scale Air Quality Model"

Ryan Schmedding<sup>1\*</sup>, Quazi Z. Rasool<sup>1\*</sup>, Yue Zhang<sup>1,4</sup>, Havala O. T. Pye<sup>1,2</sup>, Haofei Zhang<sup>3</sup>,

Yuzhi Chen<sup>1</sup>, Jason D. Surratt<sup>1</sup>, Ben H. Lee<sup>5</sup>, Claudia Mohr<sup>5,8</sup>, Felipe D. Lopez-Hilfiker<sup>5,9</sup>, Joel A. Thornton<sup>5</sup>, Allen H. Goldstein<sup>6,7</sup> and William Vizuete<sup>1€</sup>

- Department of Environmental Science and Engineering, The University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, 27516
- National Exposure Research Laboratory, Office of Research and Development, Environmental Protection Agency, Research Triangle Park, Durham, North Carolina, 27709
- 3. Department of Chemistry, University of California at Riverside, Riverside, California, 92521

4. Aerodyne Research, Inc., Billerica, Massachusetts, 01821

- 5. Department of Atmospheric Sciences, University of Washington, Seattle, WA 98195
- 6. Department of Environmental Science, Policy, and Management, University of California,

## Berkeley, CA 94720

7. Department of Civil and Environmental Engineering, University of California, Berkeley, CA

## 94720

 Present address: Department of Environmental Science and Analytical Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden.

9. Present address: Tofwerk AG, CH-3600 Thun, Switzerland.

\* Shared lead authorship

<sup>€</sup>Corresponding author: e-mail: vizuete@unc.edu; Telephone: +1 919-966-0693; Fax: +1 919-966-7911



**Figure S1** – Diurnal pattern for SOAS (June 1- July 15) 2013 of the contributions of aerosol liquid water (green) to Organic glass transition temperature  $(T_{org})$  (gray) at the (**A**) Centreville, AL site and the (**B**) Jefferson Street, Atlanta site. Bars/shading indicate 25<sup>th</sup> to 75<sup>th</sup> percentiles. Lines indicate means.



**Figure S2** – For Southeastern United States, Probability distribution of  $\gamma_{\text{IEPOX}}$  at the surface level for the *NonPhaseSep* (red), *PhaseSep* (green) for SOAS 2013 simulation period.



**Figure S3** – Average organic coating thickness (*l*<sub>org</sub> in nm) at the surface level for *PhaseSep* case for SOAS 2013 simulation period.



**Figure S4** – Average fraction of IEPOX-derived SOA in biogenic SOA mass at the surface level for: **(A)** *NonPhaseSep and* **(B)** *PhaseSep* case for SOAS 2013 simulation period.



**Figure S5** – Spatial map of the mean percent relative change of PM<sub>2.5</sub> organic carbon (OC) mass in *PhaseSep* case relative to the *NonPhaseSep* Simulation.







**Figure S6** – PM<sub>2.5</sub> organic carbon (OC) mass ( $\mu$ g/m<sup>3</sup>) as a function of hour of the day. Nonaggregated performance statistics- Mean Bias ( $\mu$ g/m<sup>3</sup>), % Normalized Mean Bias (NMB) and Spearman's Correlation coefficient (r<sup>2</sup>) of *NonPhaseSep* (green) and *HighHorg* (blue) relative to

observed (grey) PM<sub>2.5</sub> OC mass: **A-** for Rural Centreville, Alabama site and, **C-** for Urban Jefferson Street, Atlanta, Georgia site. Non-aggregated performance statistics *NonPhaseSep* (green) and *PhaseSep2* (blue) cases relative to observed (grey) PM<sub>2.5</sub> OC mass: **B-** for Rural Centreville, Alabama site and, **D-** for Urban Jefferson Street, Atlanta, Georgia site). Bars/shading indicate 25<sup>th</sup> to 75<sup>th</sup> percentiles. Lines indicate means. n= number of observation points.



**Figure S7** – Spatial map of the mean percent relative change of PM<sub>2.5</sub> sulfate mass in *Emission Reduction* sensitivity case relative to the *PhaseSep* Simulation.