

Supplemental Information

Simulation of Atmospheric Organic Aerosol using its Volatility-Oxygen Content Distribution during the PEGASOS 2012 campaign

Eleni Karnezi^a, Benjamin N. Murphy^b, Laurent Poulain^c, Hartmut Herrmann^c, Alfred Wiedensohler^c, Florian Rubach^{c,d,e}, Astrid Kiendler-Scharr^d, Thomas F. Mentel^d and Spyros N. Pandis^{a,f,g*}

^a Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, USA

^b National Exposure Research Laboratory, United States Environmental Protection Agency, Research Triangle Park, North Carolina, USA

^c Leibniz Institute for Tropospheric Research, Permoserstr 15, 04318 Leipzig, Germany

^d Institut für Chemie und Dynamik der Geosphäre, ICG, Forschungszentrum Jülich, Jülich, Germany

^e Max Planck Institute for Chemistry, 55128 Mainz, Germany

^f Department of Chemical Engineering, University of Patras, Patra, Greece

^g Inst. of Chemical Engineering Sciences, FORTH/ICEHT, Patra, Greece

Table S1. Performance of simulations with various vaporization enthalpies for the 1-bin parameterization during PEGASOS campaign for O:C measurements at the ground.

Simulation	Measured Average	Predicted Average	Fractional Error	Fractional Bias	Absolute Error	Absolute Bias
1-bin with $\Delta H_{\text{vap}}=30$ kJ mol^{-1}	0.58	0.64	0.14	0.10	0.09	0.06
1-bin with $\Delta H_{\text{vap}}=75$ kJ mol^{-1}		0.62	0.12	0.07	0.07	0.04
1-bin with $\Delta H_{\text{vap}}=150$ kJ mol^{-1}		0.59	0.11	0.02	0.06	0.007



Figure S1. The path that the Zeppelin followed during one representative day (July 4, 2012), over the Po Valley in Italy.

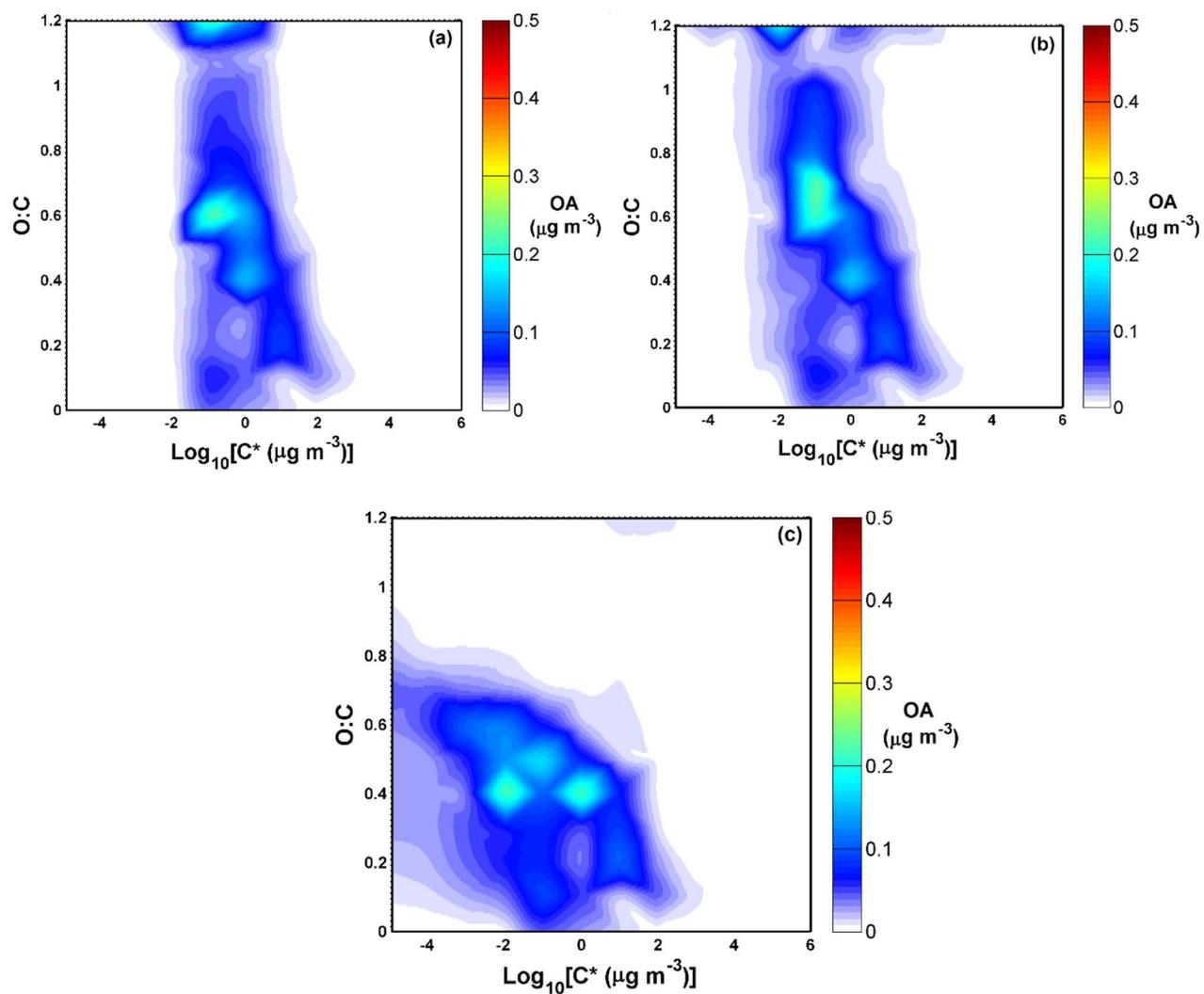


Figure S2. Average O:C-volatility distribution of OA mass concentration on San Pietro Capofiume using (a) the simple scheme (1-bin), (b) the two-bin shift simple scheme (2-bin) and (c) the detailed functionalization scheme (DET).

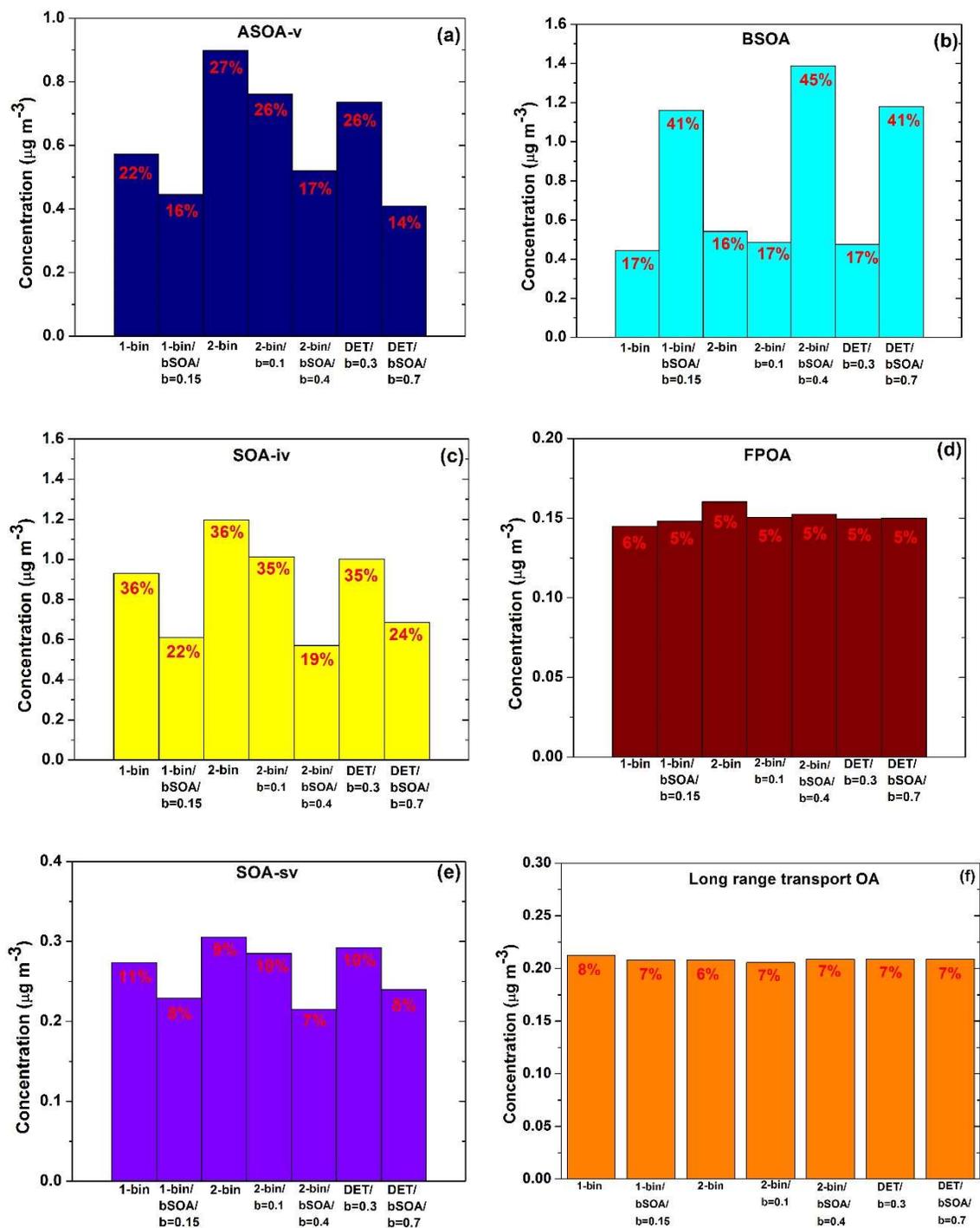


Figure S3. Predicted contribution of (a) ASOA-v, (b) bSOA, (c) SOA from oxidation of intermediate volatility organic compounds (SOA-iv), (d) FPOA, (e) SOA from oxidation of evaporated POA, and (f) OA from long range transport for the various aging parameterizations.

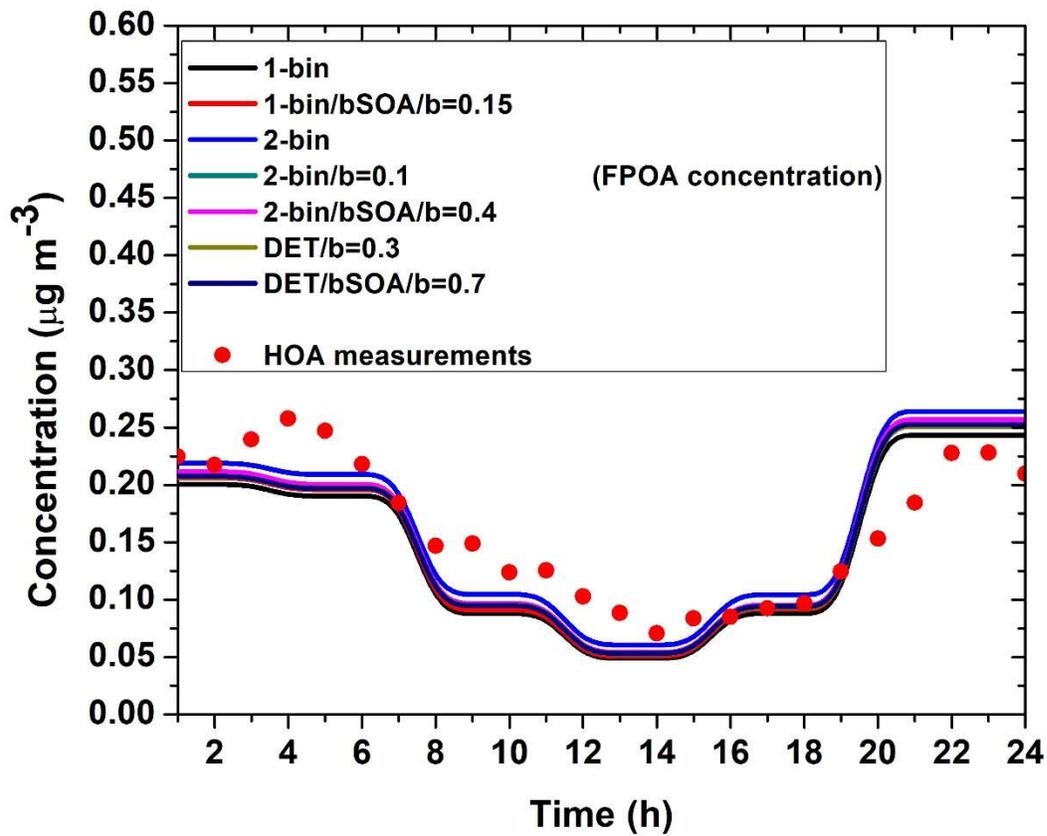


Figure S4. Average diurnal profile at the ground for POA concentration using various parameterizations (with the colored lines) and average diurnal HOA concentration from the PMF-AMS measurements with the red symbols.

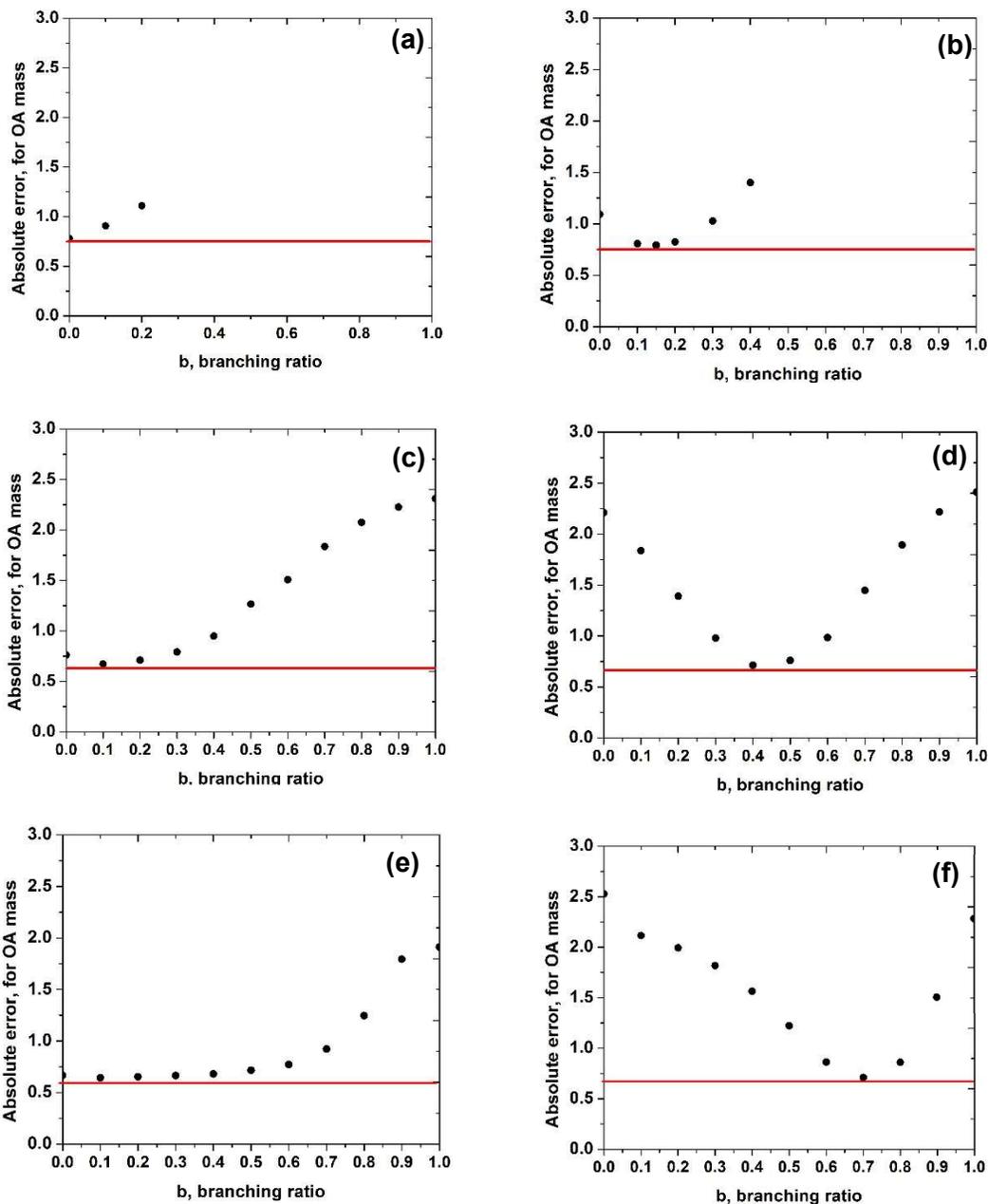


Figure S5. Estimation of optimum branching ratio (fragmentation probability) for fragmentation for the: (a) simple functionalization (1-bin), (b) simple functionalization with bSOA aging (1-bin/bSOA), (c) 2-bin functionalization (2-bin), (d) 2-bin functionalization with bSOA aging (2-bin/bSOA), (e) detailed functionalization scheme (DET) and (f) detailed functionalization with bSOA aging (DET/bSOA). The red line shows the minimum absolute error. Note that for the first case of 1-bin parameterization the optimum is at $b=0$.

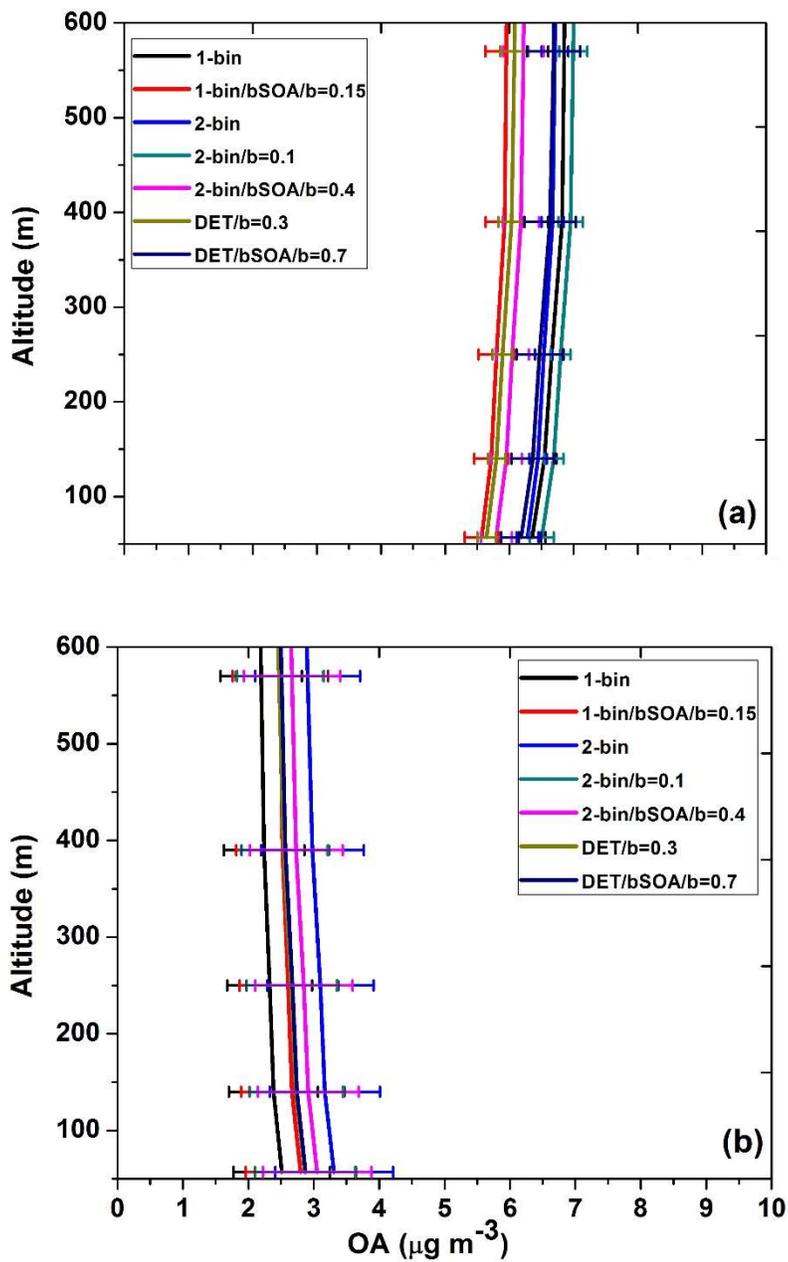


Figure S6. Averaged vertical profiles for (a) O:C ratio and (b) OA mass concentration using various parameterizations.