Supplement of Atmos. Chem. Phys., 18, 10759–10772, 2018
https://doi.org/10.5194/acp-18-10759-2018-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Simulation of atmospheric organic aerosol using its volatility–oxygen-content distribution during the PEGASOS 2012 campaign

Eleni Karnezi et al.

Correspondence to: Spyros Pandis (spyros@chemeng.upatras.gr)

Equations for metrics

$$Fractional\ Error = \frac{2}{n}\sum_{i=1}^{n}\frac{\left|P_i - M_i\right|}{\left(P_i + M_i\right)}$$

$$Fractional\ Bias = \frac{2}{n}\sum_{i=1}^{n}\frac{\left(P_i - M_i\right)}{\left(P_i + M_i\right)}$$

$$Absolute\ Error = \frac{1}{n}\sum_{i=1}^{n}\left|P_i - M_i\right|$$

$$Absolute\ Bias = \frac{1}{n}\sum_{i=1}^{n}\left(P_i - M_i\right)$$

$$Root\ Mean\ Square\ Error = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(P_i - M_i\right)^2}$$

where P_i represents the model prediction value, M_i is the corresponding measured value from the ground or above the site with the Zeppelin measurements and n is the total number of data points.

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 ΔH_{vap}= 30 kJ mol^{-1}	0.58	0.64	0.14	0.10	0.09	0.06
1-bin with ΔH_{vap}= 75 kJ mol^{-1}		0.62	0.12	0.07	0.07	0.04
1-bin with ΔH_{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.

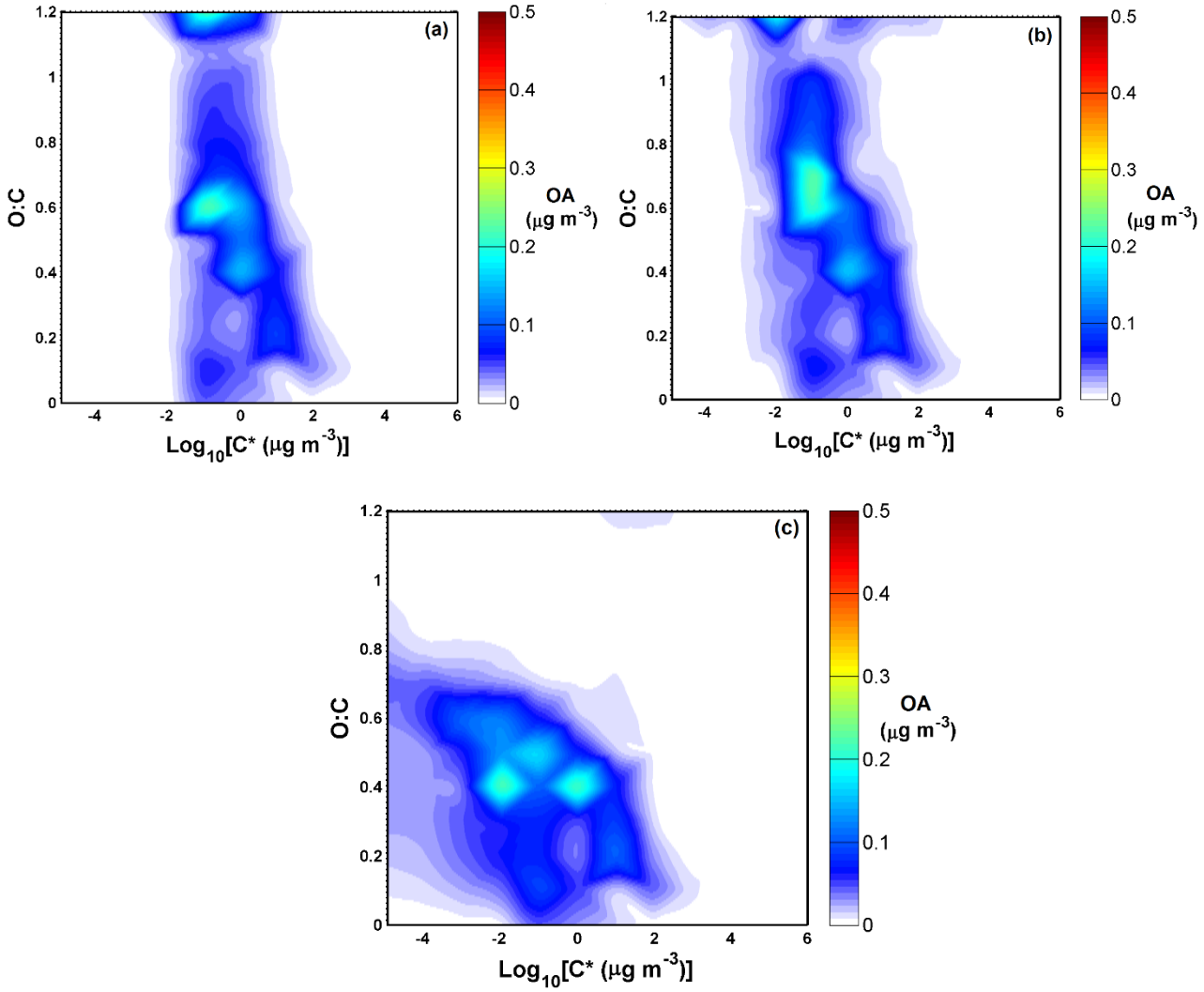

Figure S2. Average O:C-volatility distribution of OA mass concentration on San Pietro Capofiume using (a) the simple scheme (1-bin), (b) the two-bin shift simple scheme (2-bin) and (c) the detailed functionalization scheme (DET).

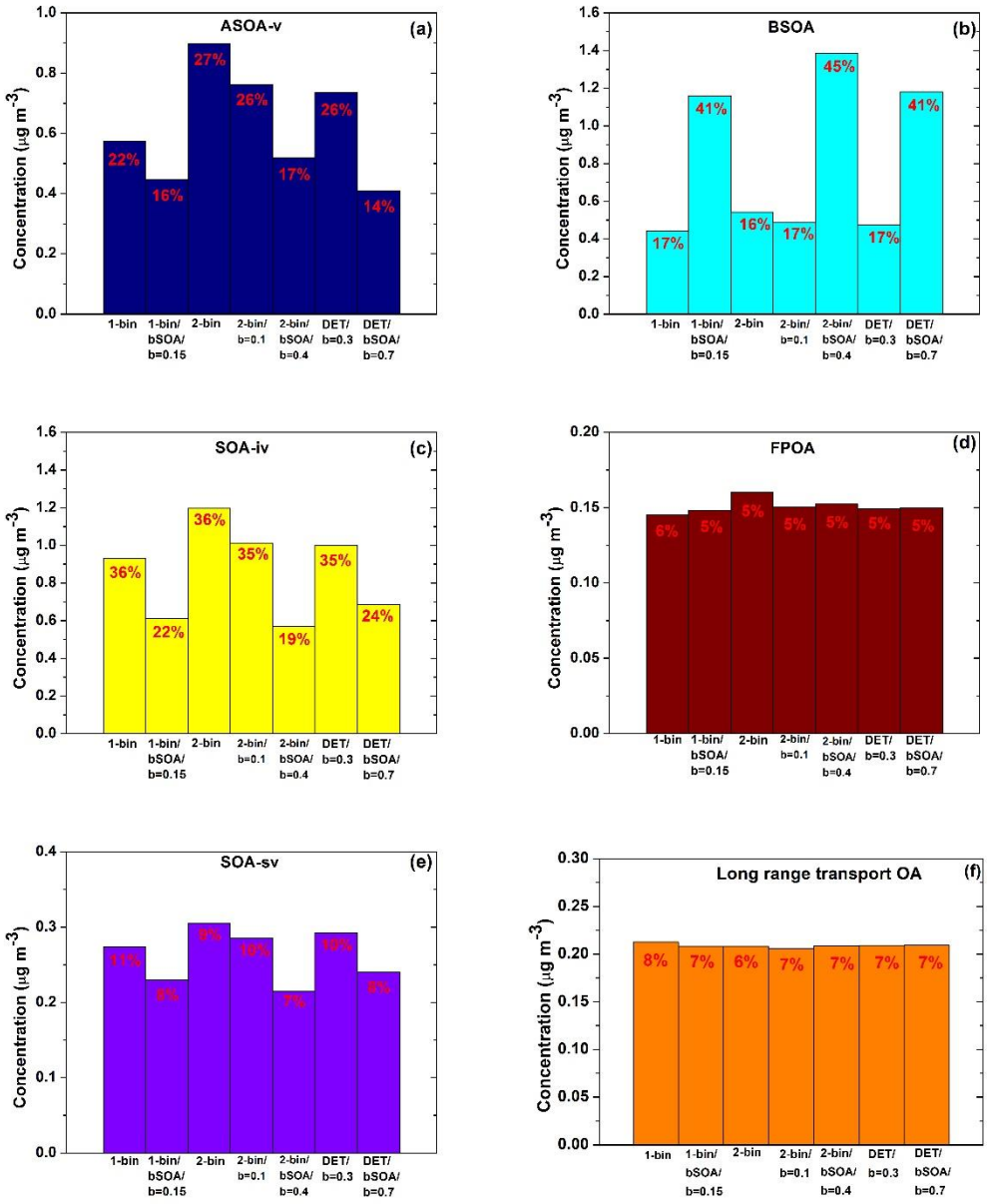

Figure S3. Predicted contribution of (a) ASOA-v, (b) bSOA, (c) SOA from oxidation of intermediate volatility organic compounds (SOA-iv), (d) FPOA, (e) SOA from oxidation of evaporated POA, and (f) OA from long range transport for the seven best performed aging parameterizations: simple functionalization (1-bin), simple functionalization with bSOA aging and b=0.15 (1-bin/bSOA/b=0.15), 2-bin functionalization (2-bin), 2-bin functionalization and b=0.1 (2-bin/b=0.1), 2-bin functionalization with bSOA aging and b=0.4 (2-bin/bSOA/b=0.4), (e) detailed functionalization scheme with b=0.3 (DET/b=0.3) and detailed functionalization with bSOA aging and b=0.7 (DET/bSOA/b=0.7).

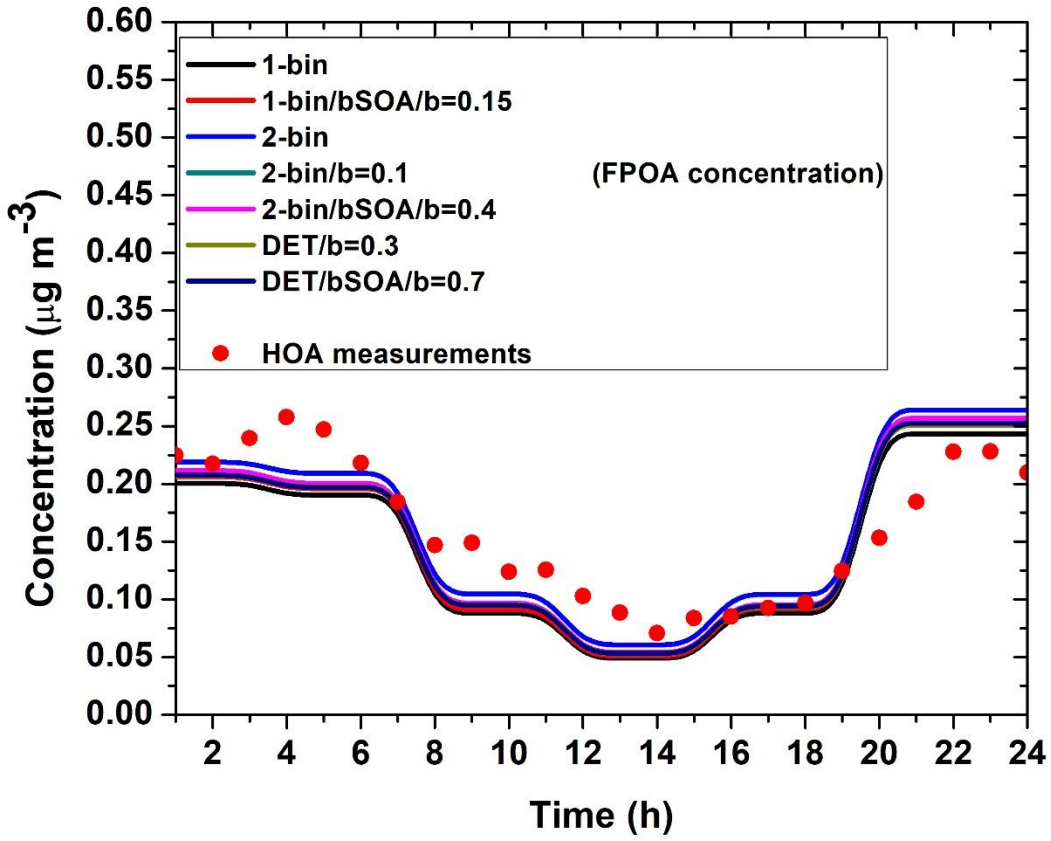

Figure S4. Average diurnal profile at the ground for POA concentration using various parameterizations (with the colored lines) and average diurnal HOA concentration from the PMF-AMS measurements with the red symbols.

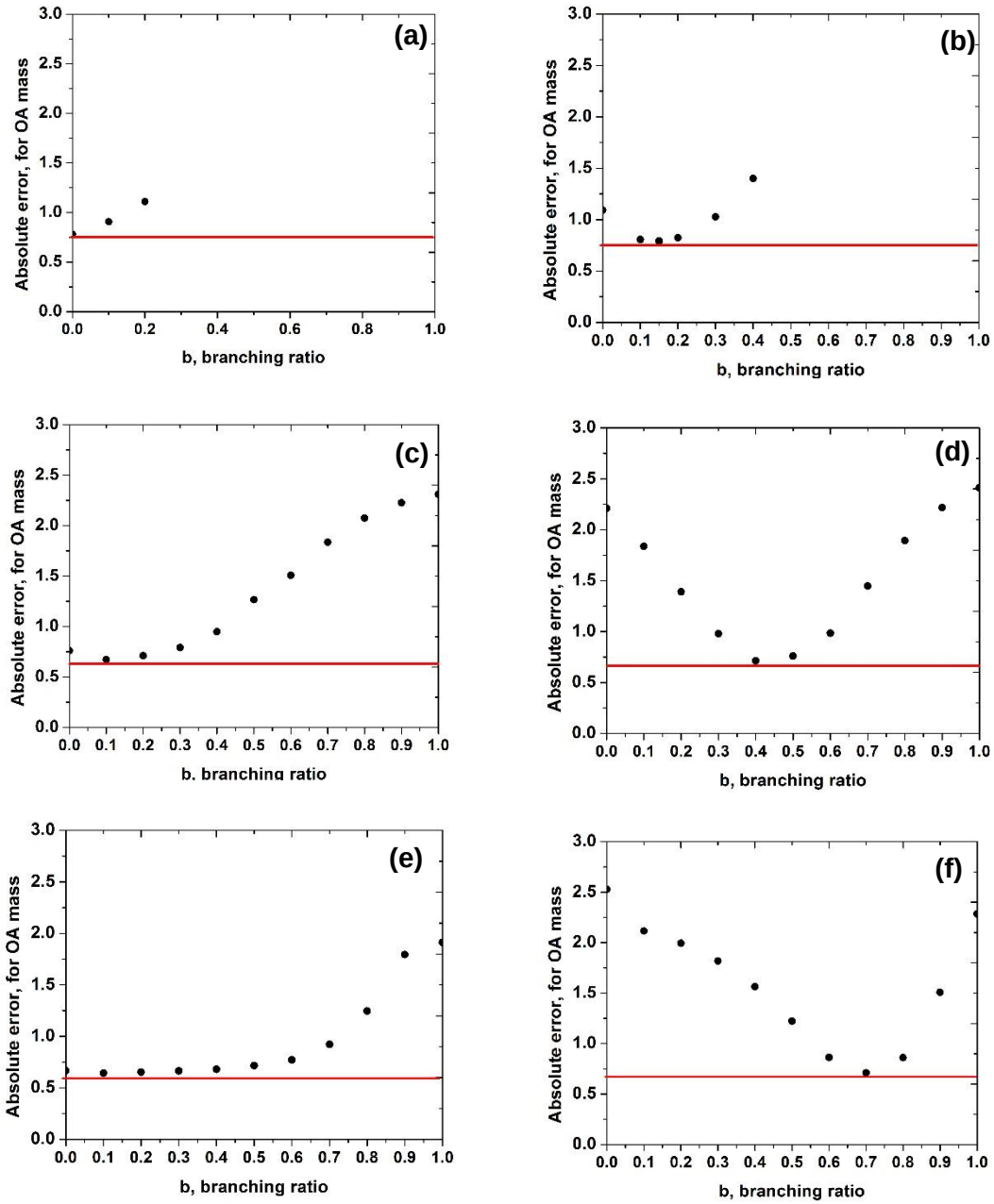

Figure S5. Estimation of optimum branching ratio (fragmentation probability) for fragmentation for the: (a) simple functionalization (1-bin), (b) simple functionalization with bSOA aging (1-bin/bSOA), (c) 2-bin functionalization (2-bin), (d) 2-bin functionalization with bSOA aging (2-bin/bSOA), (e) detailed 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.

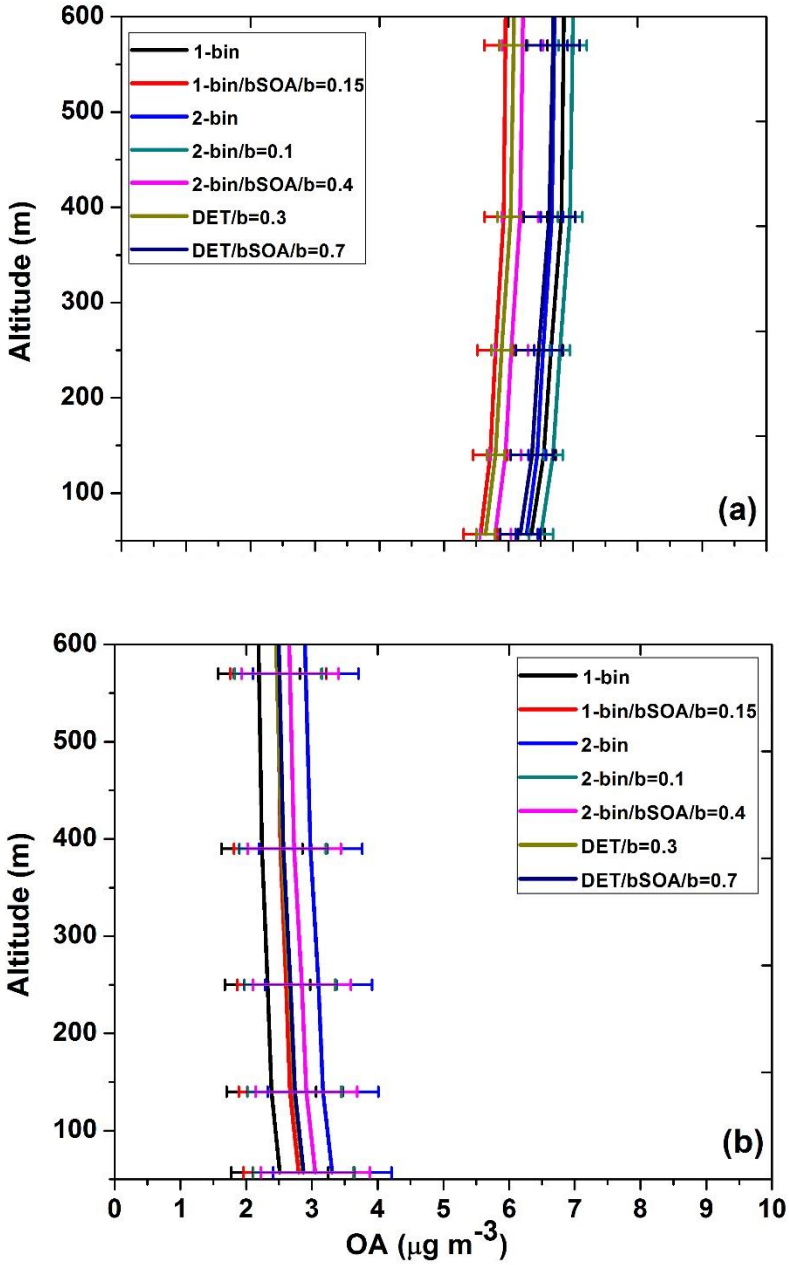

Figure S6. Averaged vertical profiles for (**a**) O:C ratio and (**b**) OA mass concentration using various parameterizations.