Supplement of Atmos. Chem. Phys., 16, 3327–3344, 2016
http://www.atmos-chem-phys.net/16/3327/2016/
doi:10.5194/acp-16-3327-2016-supplement

Atmospheric Chemistry and Physics Open Access EGU

Supplement of

Molecular corridors and parameterizations of volatility in the chemical evolution of organic aerosols

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Table S1 shows the best-fit parameters for the following equation including the contribution of the number of hydrogen atoms to the saturation mass concentration. Comparing Fig. 3 and Fig. S1 as well as Fig. 4 and Fig. S2, we found that inclusion of the number of hydrogen atoms (Eq. S1) could improve the prediction for compounds in the CH class but has only slight impact on the prediction for compounds in other composition classes.

$$\log_{10}C_{\mathrm{o}} = (n_{\mathrm{C}}^{0} - n_{\mathrm{C}})b_{\mathrm{C}} - n_{\mathrm{O}}b_{\mathrm{O}} - n_{\mathrm{H}}b_{\mathrm{H}} - 2\frac{n_{\mathrm{C}}n_{\mathrm{O}}}{n_{\mathrm{C}}+n_{\mathrm{O}}}b_{\mathrm{CO}} - n_{\mathrm{N}}b_{\mathrm{N}} - n_{\mathrm{S}}b_{\mathrm{S}} \quad (1)$$

Table S1. Composition classes and the n_C^0 and b values for saturation mass concentration parameterizations (Eq. S1) obtained by least-squares optimization using the NCI database.

Classes	n_{C}^{0}	b_{C}	b_{H}	b_{O}	b_{CO}	b_{N}	b_{S}
CH	17.95	0.5742	-0.1417				
CHO	15.77	0.6238	-0.1387	1.735	-0.8592		
CHN	23.01	0.4307	-0.02110			0.9528	
CHON	21.12	0.4139	-0.03760	0.8092	-0.1174	1.1010	
CHOS	16.07	0.5348	-0.1507	1.354	-0.4175		0.8993
CHONS	19.20	0.5469	-0.1368	1.183	0.07310	1.0289	1.323

Table S2. Statistics for comparison of the saturation mass concentration of nitrogen- and sulfur-containing compounds predicted by the EPI Suite (E) and the Eq. (2) (P).

	Number	Median_E[a]	Median_P[b]	Mean_E[c]	Mean_P[d]	MB[e]	MAGE[f]	R[g]
CHN compounds								
Primary amine	222	4.92	4.82	4.38	4.17	-0.21	0.92	0.93
Secondary amine	322	3.94	3.75	3.80	3.27	-0.53	0.96	0.94
Tetiary amine	473	3.22	2.23	3.01	1.80	-1.21	1.35	0.93
Quaternary amine	158	-2.55	2.05	-3.38	2.04	5.42	5.42	0.86
Heterocyclic ring	1209	1.35	1.53	1.27	1.32	0.05	1.03	0.88
Imine	249	1.00	0.35	0.52	0.07	-0.45	1.23	0.93
Nitriles	282	3.53	3.60	3.41	3.35	-0.06	0.74	0.93
CHON compounds								
Amide	5117	-0.10	0.47	-0.49	-0.11	0.41	1.67	0.84
Imine	741	0.35	-0.09	-0.37	-0.66	-0.29	1.78	0.89
Primary amine	576	2.74	2.78	2.57	2.36	-0.21	1.53	0.70
Secondary amine	748	1.10	0.87	0.78	0.55	-0.23	1.40	0.85
Tetiary amine	2130	0.63	-0.42	0.26	-0.54	-0.80	1.67	0.85
Quaternary amine	225	-4.05	-0.23	-4.65	-0.65	4.00	4.00	0.86
Nitroso	15	3.95	2.78	3.80	2.57	-1.23	1.29	0.82
Nitro	750	2.18	0.71	1.92	0.35	-1.56	1.76	0.88
Organonitrate	9	3.50	0.30	3.06	0.70	-2.36	2.86	0.94
Alkyl nitrite	3	8.39	4.58	8.00	4.46	-3.54	3.54	0.99
Azole	425	-0.24	-0.52	-1.27	-1.24	0.04	1.79	0.84
Pyrimidine	1600	0.68	0.30	0.26	-0.08	-0.34	1.40	0.84
Purine	369	-1.38	-1.65	-2.82	-2.56	0.56	1.69	0.86
Amino acid	400	-1.52	2.05	-1.54	1.63	-3.17	3.30	0.62
nitrile	356	2.38	1.40	2.23	1.01	-1.21	1.64	0.81
CHOS compounds								
Organosulfate	17	1.45	1.90	-0.87	0.14	1.01	1.42	0.98
Sulfonate	295	-1.25	-0.79	-2.05	-1.33	0.73	2.25	0.82
Sulfone	173	1.33	0.86	1.16	0.76	-0.40	0.92	0.89
Sulfoxides	12	1.52	2.30	2.38	2.82	0.45	0.88	0.94
Sulfite	7	5.64	3.14	5.45	2.89	-2.56	2.56	0.95
CHONS compounds								
Organosulfate	8	-4.01	-2.42	-4.03	-2.80	1.23	1.52	0.96
Sulfonate	601	-8.65	-7.44	-10.94	-10.41	1.79	2.22	0.97
Sulfone	85	-2.12	-4.42	-3.70	-5.95	-1.66	2.09	0.94
Sulfonamide	648	-1.03	-2.72	-1.67	-3.35	-1.67	1.91	0.91
Organic amide	178	-3.27	-3.43	-4.08	-4.21	-0.12	1.66	0.93
Thioamide	244	-0.21	-0.85	-0.74	-1.54	-0.80	1.49	0.87
Heterocyclic ring	1315	-1.15	-0.89	-1.98	-1.68	0.33	1.55	0.90
Amino acid	45	-1.98	1.35	-1.54	0.92	2.47	2.57	0.91
Thioate	58	0.30	-0.28	-0.28	-1.56	-1.28	1.94	0.86
thiocarbamate	36	-2.67	-1.55	-3.64	-2.44	1.20	1.62	0.92

[a]Median $\log_{10}(C_o)$ predicted by the EPI Suite.

[b]Median $\log_{10}(C_o)$ predicted by the Eq. (2).

[c]Mean $\log_{10}(C_o)$ predicted by the EPI Suite.

[d]Mean $\log_{10}(C_o)$ predicted by the Eq. (2).

[e]Mean bias.

[f]Mean absolute gross error.

[g]Correlation coefficient.

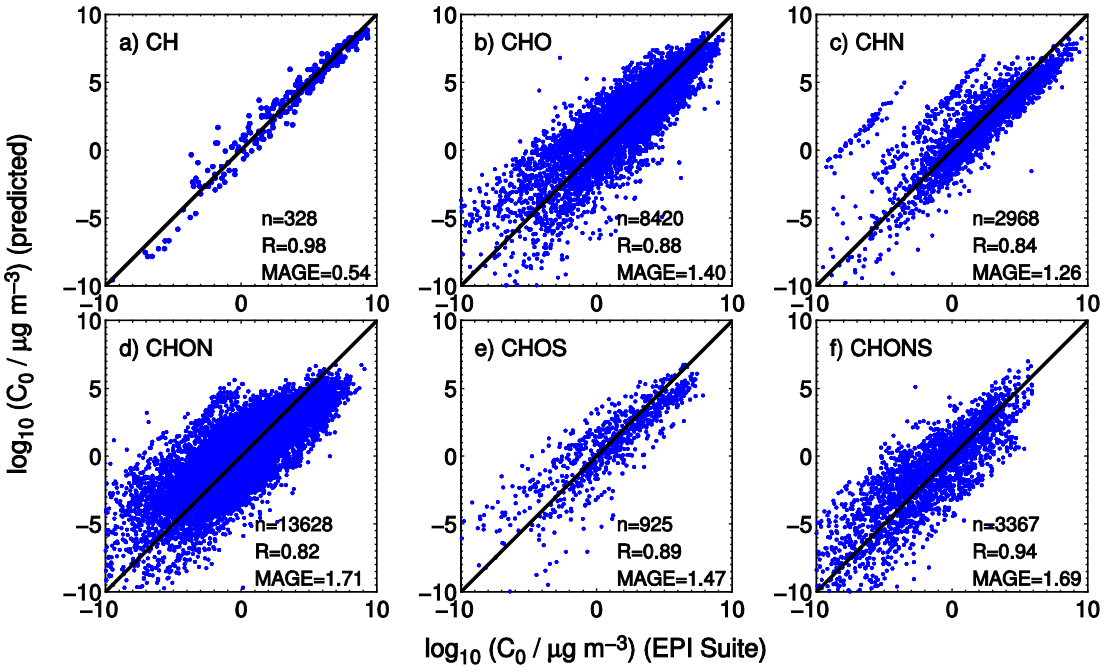

Figure S1. Saturation mass concentration (C_0) of organic compounds predicted by Eq. S1 using the parameters in Table S1 plotted against C_0 determined by the EPI Suite software in the NCI database for elemental composition classes of **(a)** CH, **(b)** CHO, **(c)** CHN, **(d)** CHON, **(e)** CHOS, and **(f)** CHONS.

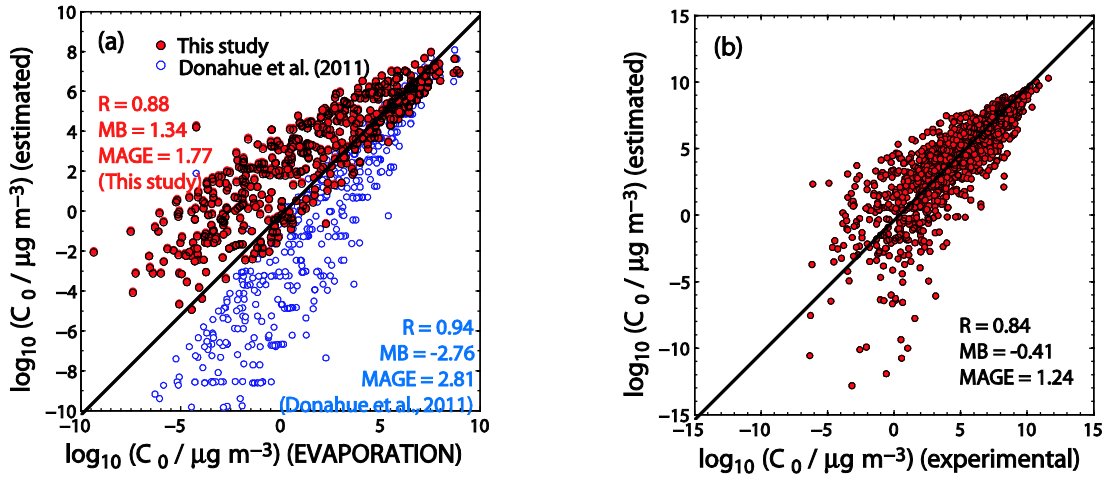

Figure S2. (a) Saturation mass concentration (C_0) of CHO compounds predicted by Eq. S1 with the coefficients in Table S1 and with the coefficients from Donahue et al. (2011) plotted against C_0 computed by the EVAPORATION model (Compernolle et al., 2011). The data comprise 704 SOA oxidation products from biogenic (isoprene, α-pinene, limonene, glyoxal) and anthropogenic precursors (C12 alkanes) as presented in Shiraiwa et al. (2014). (b) Comparison of C_0 predicted by Eq. S1 with the coefficients in Table S1 and experimental values taken from PHYSPROP database (http://esc.syrres.com/interkow/EpiSuiteData.htm).