

# Supplementary Material for: A Comparison of the chemical sinks of atmospheric organics in the gas and aqueous phase

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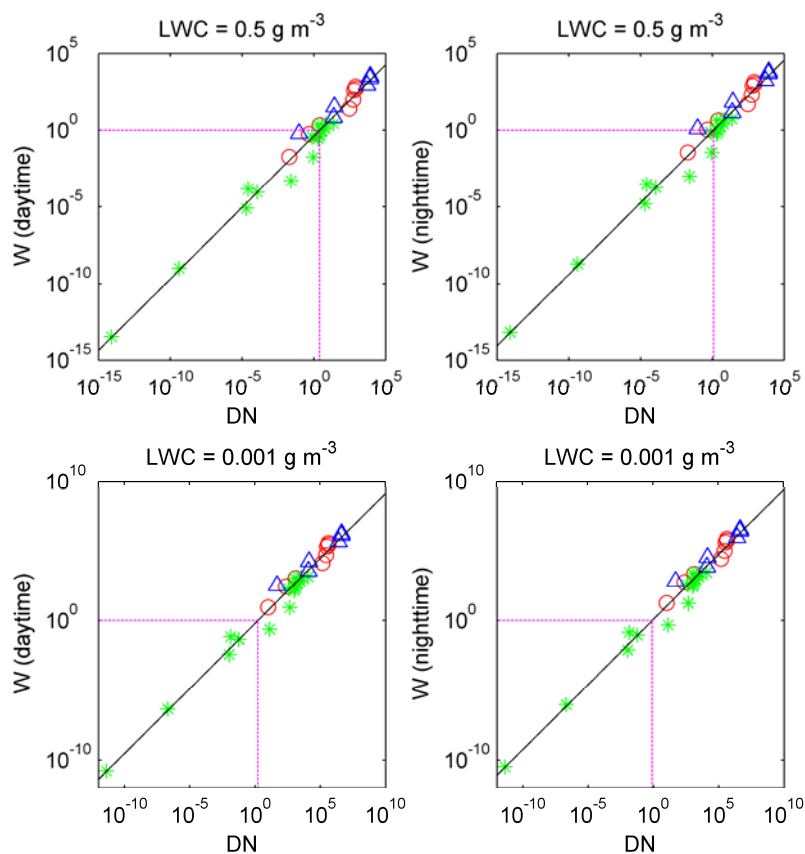


Figure S1. The ratio of the rate of gas phase OH oxidation to the rate of aqueous phase oxidation,  $W$ , as a function of the dimensionless number,  $DN = \frac{1}{10}(LWC_v \cdot R \cdot T \cdot k_H)^{-1}$  for the

series of compounds investigated at 298 K. Upper left panel: daytime OH conditions with  $LWC = 0.5 \text{ g m}^{-3}$ . Upper right panel: nighttime OH conditions with  $LWC = 0.5 \text{ g m}^{-3}$ . Lower left panel: daytime OH conditions with  $LWC = 0.001 \text{ g m}^{-3}$ . Upper right panel: nighttime OH conditions with  $LWC = 0.001 \text{ g m}^{-3}$ . The magenta dashed line indicates the transition between gaseous reactions being more important,  $DN \gg 1$  and aqueous reactions being more important,  $DN \ll 1$ .

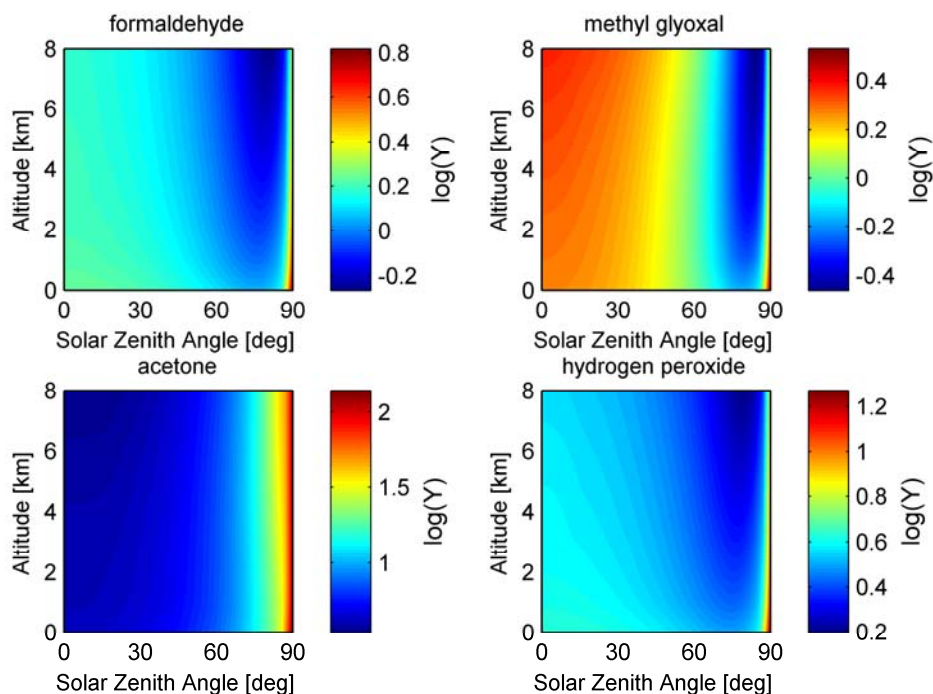


Figure S2: Upper bound for the ratio of the rate of gas phase OH oxidation to the rate of gaseous photolysis,  $Y$ , as a function of solar zenith angle and altitude for compounds where the absorption cross sections and quantum yields are published as a function of temperature and pressure. Rohrer and Berresheim (Rohrer and Berresheim, 2006) use five field missions to fit their correlation between OH concentration and  $O_3$  photolysis. This analysis uses the maximum predicted OH values from their correlation.

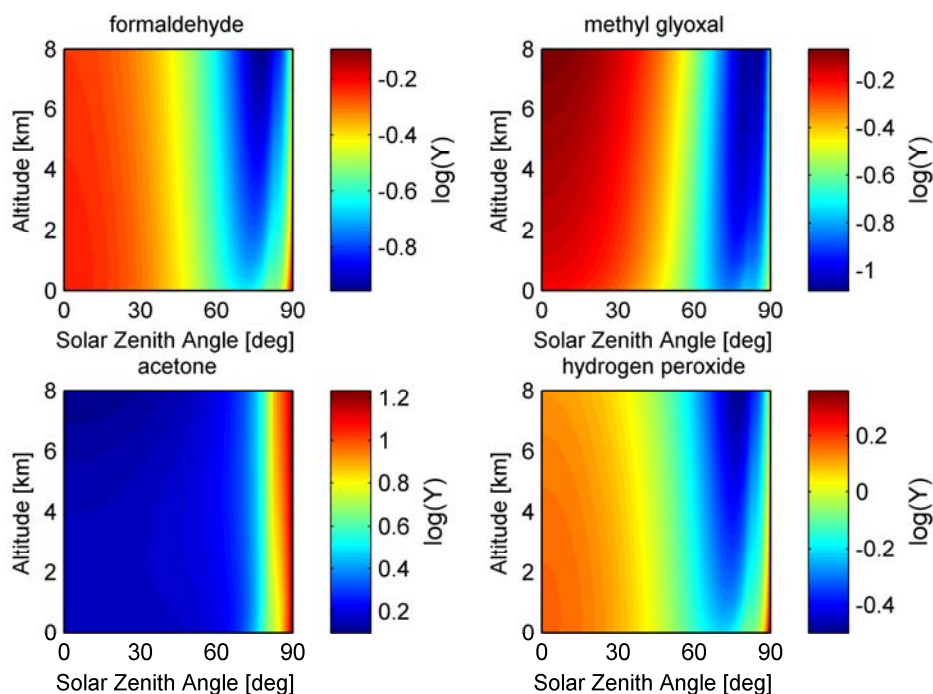


Figure S3: Lower bound for the ratio of the rate of gas phase OH oxidation to the rate of gaseous photolysis,  $Y$ , as a function of solar zenith angle and altitude for compounds where the absorption cross sections and quantum yields are published as a function of temperature and pressure. Rohrer and Berresheim (Rohrer and Berresheim, 2006) use five field missions to fit their correlation between OH concentration and  $O_3$  photolysis. This analysis uses the minimum predicted OH values from their correlation.

Table S1: List of aqueous and gas phase rate constants and their references. “NAV” indicates that data were not available in the literature and “NA” indicates that the particular value is not applicable to the species of interest. Henry’s law constants obtained from theoretical estimations are indicated by an asterisk in the “kH Reference” column. In cases where measurements exist from multiple researchers and an agreed value was not established, we used the mean of the experimental values. “SAR” indicates that the given value was predicted theoretically based on structure from (Kwok and Atkinson, 1995). Acid dissociation constants were obtained from (Serjeant and Dempsey, 1979; Perrin et al., 1981; Gligorovski et al., 2009; Perrin, 1965). Hydration equilibrium constants were obtained from (Malik and Joens, 2000; Dong and Dasgupta, 1986; Bell and McDougall, 1960; Nemet et al., 2004; Betterton and Hoffmann, 1988)

Molecule	CAS	kH at 298 K [M/atm]	kH(T) "B value"	kH Reference	kOHliq (1/s/M)	kOHliq Anion (1/s/M)	kOHliq Ref	kOHgas (mol/cm <sup>3</sup> /s)	kOHgas Ref	Gas Photo. Ref
formic acid	64-18-6	8.90E+03	6100	Sander, S.P. 2011	1.00E+08	2.40E+09	Ervens 2003	4.38333E-13	NIST Kinetics	NAV
acetic acid	64-19-7	4.10E+03	6200	Sander, S.P. 2011	1.70E+07	7.00E+07	Ervens 2003	7.56333E-13	NIST Kinetics	NAV
propanoic acid	79-09-4	4.10E+03	NAV	Sander, R. 1999	3.20E+08	8.90E+08	Ervens 2003	1.20E-12	NIST Kinetics	NAV
2-methyl propanoic acid	79-31-2	3.40E+03	NAV	Sander, R. 1999	NAV	NAV	Buxton 1988	2.06E-12	NIST Kinetics	NAV
pentanoic acid	109-52-4	2.20E+03	6741.5	Sander, R. 1999	NAV	2.90E+09	Buxton 1988	6.75E-12	SAR	NAV
3-methyl butanoic acid	503-74-2	1.20E+03	NAV	Sander, R. 1999	4.30E+08	2.40E+09	NIST	8.85E-12	SAR	NAV
2,2-dimethyl 1-propanoic acid	75-98-9	3.50E+02	NAV	Sander, R. 1999	6.50E+08	1.50E+09	NIST	1.69E-12	SAR	NAV
hexanoic acid	142-62-1	1.40E+03	6304	Sander, R. 1999	NAV	4.00E+09	Buxton 1988	8.16E-12	SAR	NAV
malonic acid	141-82-2	4.00E+08	NAV	Sander, R. 1999*	1.60E+07	1.90E+08	NIST	7.19E-13	SAR	NAV
succinic acid	110-15-6	3.00E+08	NAV	Sander, R. 1999*	5.00E+08	1.10E+08	Ervens 2003	5.60E-12	SAR	NAV
glyoxal	107-22-2	4.19E+05	7480	Sander, S.P. 2011	1.10E+09	NA	Buxton 1997	9.70E-12	NIST Kinetics	Sander, S.P. 2011
formaldehyde	50-00-0	3.23E+03	7100	Sander, S.P. 2011	1.00E+09	NA	Buxton 1988	8.50E-12	Sander, S.P. 2011	NAV
acetaldehyde	75-07-0	1.29E+01	5890	Sander, S.P. 2011	2.40E+09	NA	Schuchmann 1988	1.50E-11	Sander, S.P. 2011	NAV
methyl glyoxal	78-98-8	1.79E+04	NAV	Sander, R. 1999	1.10E+09	NA	Ervens 2003	1.30E-11	NIST Kinetics	Atkinson 2006
propanal	123-38-6	1.00E+01	4330	Sander, S.P. 2011	2.20E+09	NA	Mezyk 19994	1.90E-11	Sander, S.P. 2011	Heicklen 1986 / Sander, S.P. 2011
butanal	123-72-8	9.60E+00	6220	Sander, S.P. 2011	3.90E+09	NA	Adams 1965	2.38E-11	NIST Kinetics	Atkinson 2006
acetone	67-64-1	2.78E+01	5050	Sander, S.P. 2011	2.10E+08	NA	Ervens 2003	1.79E-13	Sander, S.P. 2011	Sander, S.P. 2011
2-butanone	78-93-3	1.50E+01	5350	Sander, R. 1999	6.60E+08	NA	Mezyk 1994	1.20E-12	NIST Kinetics	Atkinson 2006
malic acid	6915-15-7	2.00E+13	NAV	Sander, R. 1999*	8.20E+08	9.7e8 mono / 8.5e8 di	Gligorovski 2009	2.30E-11	SAR	NAV
lactic acid	50-21-5	7.00E+07	NAV	Sander, R. 1999*	4.30E+08	8.20E+08	NIST/Logan 1989	6.20E-12	SAR	NAV
tartaric acid (R,R)	87-69-4	1.00E+18	NAV	Sander, R. 1999*	7.00E+08	1.10E+09	NIST/Logan 1989	4.05E-11	SAR	NAV
hydrogen peroxide	7722-84-1	8.44E+04	7600	Sander, S.P. 2011	2.72E+07	NA	NIST	1.70E-12	Sander, S.P. 2011	Sander, S.P. 2011
methyl peroxide	3031-73-0	3.00E+02	5280	Sander, S.P. 2011	6.05E+08	NA	Monod 2007	7.40E-12	Sander, S.P. 2011	Sander, S.P. 2011
methyl nitrate	598-58-3	2.00E+00	4700	Sander, S.P. 2011	NAV	NA	NAV	1.88E-13	NIST Kinetics	Sander, S.P. 2011
dimethyl ether	115-10-6	1.00E+00	NAV	Sander, S.P. 2011	1.00E+09	NA	NIST	2.98E-12	Atkinson 1985	NAV
methyl tert-butyl ether	1634-04-4	1.60E+00	7700	Sander, R. 1999	1.60E+09	NA	NIST	2.65E-12	Atkinson 1985	NAV
diethyl ether	60-29-7	9.30E-01	5300	Sander, R. 1999	3.55E+09	NA	NIST	1.34E-11	Atkinson 1985	NAV
glycolaldehyde	141-46-8	4.10E+03	4600	Sander, R. 1999	NAV	NAV	NAV	1.10E-11	JPL	Sander, S.P. 2011
glutaraldehyde	111-30-8	3.07E+04	NAV	Olson 1998	NAV	NAV	NAV	2.375E-11	NIST Kinetics	NAV
glyceraldehyde	367-47-5	2.00E+10	NAV	Saxena 1996*	NAV	NAV	NAV	4.05E-11	SAR	NAV
pyruvic acid	127-17-3	3.10E+05	5100	Sander, S.P. 2011	1.20E+08	7.00E+08	Ervens 2003	1.24E-13	NIST Kinetics	NAV
glyoxylic acid	279-12-4	1.09E+04	4810	Sander, S.P. 2011	3.60E+08	2.60E+09	Ervens 2003	1.28E-11	SAR	NAV

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