Supplement of Atmos. Chem. Phys., 18, 9823–9830, 2018
https://doi.org/10.5194/acp-18-9823-2018-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Technical note: Updated parameterization of the reactive uptake of glyoxal and methylglyoxal by atmospheric aerosols and cloud droplets

Leah A. Curry et al.

Correspondence to: V. Faye McNeill (vfm2103@columbia.edu)

Supporting information for

Technical note: Updated parameterization of the reactive uptake of glyoxal and methylglyoxal by atmospheric aerosols and cloud droplets

Leah A. Curry, William G. Tsui, V. Faye McNeill

Department of Chemical Engineering, Columbia University, New York, NY, 10027, USA

Correspondence to: V. Faye McNeill (vfm2103@columbia.edu)

Table S1. GEOS-Chem cloud and aerosol parameters

Cloud type	Effective radius (μm)
Liquid cloud droplet (marine)	10
Liquid cloud droplet (continental)	6

Aerosol type	Dry radius R_{dry} (μm)	Effective radius R_{eff} (μm)	Growth factor of R_{eff} (R_{eff} / $R_{eff, RH=0\%}$)	Notes
Sulfate + nitrate + ammonium	0.069	0.121 (RH = 0%); 0.149 (RH = 50%); 0.162 (RH = 70%); 0.174 (RH = 80%); 0.198 (RH = 90%); 0.227 (RH = 95%); 0.304 (RH = 99%)	1.00 (RH = 0%); 1.23 (RH = 50%) 1.34 (RH = 70%) 1.44 (RH = 80%) 1.64 (RH = 90%) 1.88 (RH = 95%) 2.51 (RH = 99%)	So4.dat based on GADS (David Ridley)
Seasalt (accumulation mode)	0.085	0.129 (RH = 0%); 0.207 (RH = 50%); 0.233 (RH = 70%); 0.256 (RH = 80%); 0.306 (RH = 90%); 0.372 (RH = 95%); 0.613 (RH = 99%)	1.00 (RH = 0%); 1.60 (RH = 50%) 1.81 (RH = 70%) 1.98 (RH = 80%) 2.37 (RH = 90%) 2.88 (RH = 95%) 4.75 (RH = 99%)	Ssa.dat based on GADS (David Ridley)
Seasalt (coarse mode)	0.401	0.952 (RH = 0%); 1.534 (RH = 50%); 1.725 (RH = 70%); 1.899 (RH = 80%); 2.274 (RH = 90%); 2.780 (RH = 95%); 4.673 (RH = 99%)	1.00 (RH = 0%); 1.61 (RH = 50%) 1.81 (RH = 70%) 1.99 (RH = 80%) 2.39 (RH = 90%) 2.92 (RH = 95%) 4.91 (RH = 99%)	Ssc.dat based on GADS (David Ridley)
Dust Bin 1		0.7 (RH >= 35%)		Dust_mod.F
Dust Bin 2		1.4 (RH >= 35%)		Dust_mod.F
Dust Bin 3		2.4 (RH >= 35%)		Dust_mod.F

Dust Bin 4		4.5 (RH >= 35%)		Dust_mod.F
Organics, hydrophilic	0.021	0.127 (RH = 0%); 0.139 (RH = 50%); 0.145 (RH = 70%); 0.149 (RH = 80%); 0.159 (RH = 90%); 0.171 (RH = 95%); 0.203 (RH = 99%)	1.00 (RH = 0%); 1.09 (RH = 50%) 1.14 (RH = 70%) 1.17 (RH = 80%) 1.25 (RH = 90%) 1.35 (RH = 95%) 1.60 (RH = 99%)	org.dat based on GADS (David Ridley)
Soot (black carbon), hydrophilic	0.020	0.035 (RH = 0%); 0.035 (RH = 50%); 0.035 (RH = 70%); 0.042 (RH = 80%); 0.049 (RH = 90%); 0.052 (RH = 95%); 0.066 (RH = 99%)	1.00 (RH = 0%); 1.00 (RH = 50%) 1.00 (RH = 70%) 1.20 (RH = 80%) 1.40 (RH = 90%) 1.49 (RH = 95%) 1.89 (RH = 99%)	soot.dat based on GADS (David Ridley)

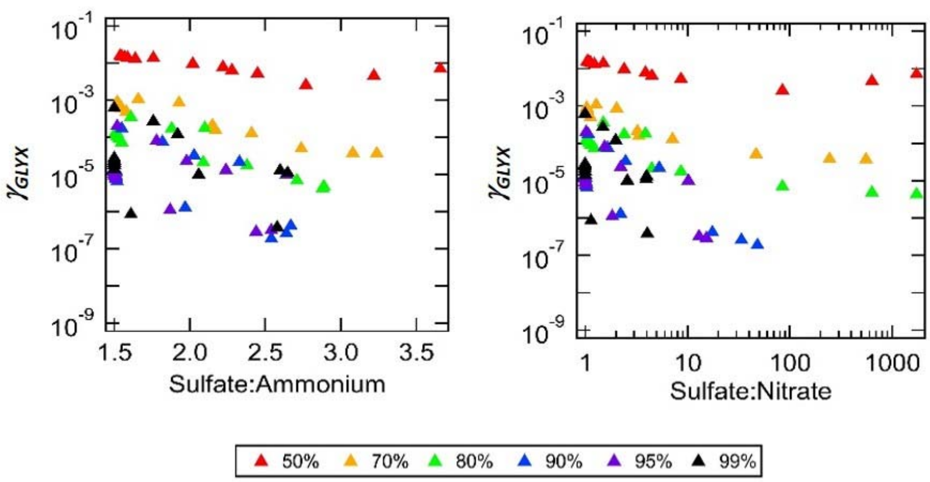

Figure S1. Calculated γ_{GLYX} as a function of aerosol composition for SNA aerosols at varying relative humidity.

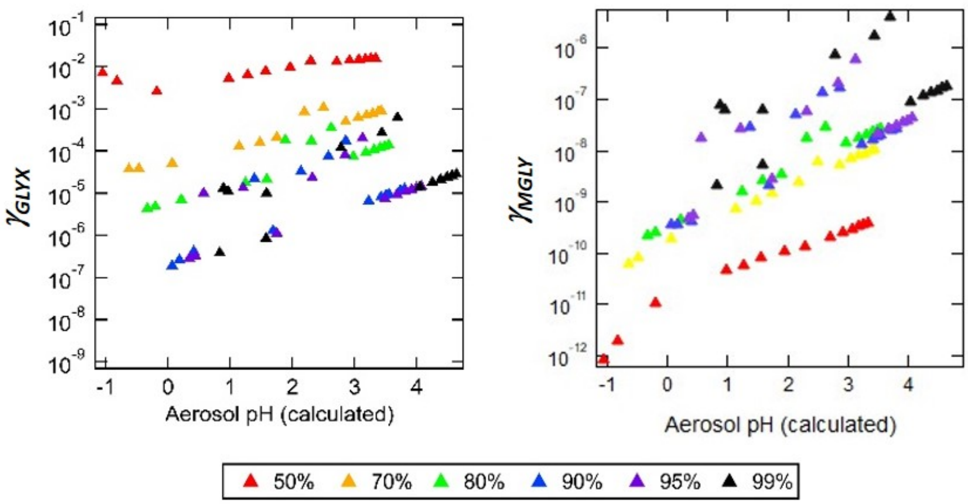

Figure S2. Calculated γ_{GLYX} and γ_{MGLY} for SNA aerosols displayed as a function of calculated aerosol pH and varying relative humidity

Table S2. Recommended parameterization of γ_{GLYX} as a function of RH and pH. For pH ≤ pH_{break}, γ_{GLYX} = exp(*a*+*b**pH). For pH > pH_{break}, γ_{GLYX} = *c*+*d**pH. Parameterization valid for -1.05 ≤ pH ≤ 4.64.

RH	pH_{break}	*a*	*b*	*c*	*d*
50%	2.30	*	*	$1.36(\pm 0.21)\times10^{-3}$	$4.31(\pm 0.07)\times10^{-3}$
70%	2.50	-9.8 ± 0.2	1.37 ± 0.05	$-1.53(\pm 0.11)\times10^{-3}$	$7.02(\pm 0.34)\times10^{-4}$
80%	2.63	-12.2 ± 0.3	1.58 ± 0.13	$-2.65(\pm 0.19)\times10^{-4}$	$1.12(\pm 0.06)\times10^{-4}$
90%	2.86	-15.6 ± 0.6	2.37 ± 0.36	$-2.81(\pm 0.20)\times10^{-5}$	$1.06(\pm 0.06)\times10^{-5}$
95%	3.13	-14.8 ± 1.0	1.84 ± 0.51	$-3.51(\pm 0.23)\times10^{-5}$	$1.21(\pm 0.06)\times10^{-5}$
99%	3.69	-14.7 ± 1.1	1.90 ± 0.48	$-8.34(\pm 0.41)\times10^{-5}$	$2.39(\pm 0.09)\times10^{-5}$

* for 50% RH, pH ≤ $pH_{break,}$ γ_{GLYX} = *a*+*b**pH+c*pH^2, where a = $3.0(\pm 0.5)\times10^{-3}$, b = $-7.4(\pm 4.5)\times10^{-4}$, and c = $2.3(\pm 0.3)\times10^{-3}$

Table S3. Recommended parameterization of γ_{MGLY} as a function of RH and pH. For pH ≤ $pH_{break,}$ γ_{MGLY} = exp(*a*+*b**pH) for pH > pH_{break}, γ_{MGLY} = *c*+*d**pH. Parameterization valid for -1.05 ≤ pH ≤ 4.64.

RH	pH_{break}	*a*	*b*	*c*	*d*
50%	2.30	-25.7 ± 0.2	1.49 ± 0.13	$-5.88(\pm 0.05)\times10^{-10}$	$2.86(\pm 0.16)\times10^{-10}$
70%	2.50	-22.7 ± 0.1	1.37 ± 0.05	$-1.95(\pm 0.13)\times10^{-8}$	$8.60(\pm 0.41)\times10^{-9}$
80%	2.63	-22.0 ± 0.2	1.58 ± 0.13	$-5.30(\pm 0.36)\times10^{-8}$	$2.21(\pm 0.11)\times10^{-8}$
90%	2.86	-22.2 ± 0.6	2.35 ± 0.35	$-5.71(\pm 0.40)\times10^{-8}$	$2.15(\pm 0.11)\times10^{-8}$
95%	3.13	-21.3 ± 1.0	2.04 ± 0.50	$-1.00(\pm 0.07)\times10^{-7}$	$3.46(\pm 0.17)\times10^{-8}$
99%	3.69	-19.9 ± 1.1	1.96 ± 0.48	$-5.07(\pm 0.32)\times10^{-7}$	$1.46(\pm 0.07)\times10^{-7}$

MATLAB routine for calculating reactive uptake coefficients

Example shown for glyoxal uptake to maritime clouds.

```
clear;

Da = 1e-9; %Gly aqueous diffusion constant, m2/s
kOH = 1.1e9; %Gly-OH bimolecular aqueous rate constant, 1/M/s
kB = 1.38e-23; %Boltzmann constant, m^2*kg/s^2/K
T = 298; % Temp, K
M = 58.04/6.023e23/1000; %% mass of one GLY molecule, kg
w = sqrt(8*kB*T/pi()/M); %m/s
alpha = 0.02;

%% Maritime CLOUD

    H = 3.6e5; %Henry's constant for dilute conditions, M/atm
    R = 10e-6; %radius, m
    OHconc = [2e-12, 5.3e-12, 3.8e-14]; % Molar

for i = 1:3
    kI=kOH*OHconc(i); % calculate psuedo first order rate constant, 1/s
    q = R*sqrt(kI/Da);
    f = coth(q)-1/q;
    gMC(i) = (1/alpha+w/(4*H*82.06/1000*T*sqrt(Da*kI))*1/f)^-1
end
```