Supplement to: Model investigation of NO_3 secondary organic aerosol (SOA) source and heterogeneous organic aerosol (OA) sink in the western United States

Juliane L. Fry and Kathryn Sackinger (Correspondence: fry@reed.edu)

Chemistry Department, Reed College, Portland, OR, USA

This supplemental information shows the experimental data used to determine average NO_3 uptake onto saturated (Table S1) and unsaturated (Table S2) organic in aerosol, the surface area of each aerosol size bin (Table S3), the carbon chain length corresponding to a given volatility bin for a molecule with specified combinations of functional groups (Table S4), and a representative WRF/Chem namelist file (Appendix).

Supplementary materials

Table S1: Uptake coefficients for nitrate radical onto saturated organic substrates

Substrate	Experimental conditions	γ	Source
Octadecanethiol monolayer	None specified	$(8.8 \pm 2.5) \times 10^{-4}$	[1]
Diethyl sebacate	298 K, liquid	$(4.1 \pm 0.3) \times 10^{-3}$	[2]
	288 K, liquid	$(3.6 \pm 0.1) \times 10^{-3}$	[2]
	278 K, liquid	$(4.1 \pm 0.5) \times 10^{-3}$	[2]
	272 K, solid	$(3.6 \pm 0.5) \times 10^{-4}$	[2]
	263 K, solid	$(2.5 \pm 0.2) \times 10^{-4}$	[2]
Glycerol	293 K, liquid	$(1.4 \pm 0.3) \times 10^{-3}$	[2]
	286 K, liquid	$(9.2 \pm 0.4) \times 10^{-4}$	[2]
	268 K, liquid	$(8.3 \pm 0.5) \times 10^{-4}$	[2]
n-hexadecane	293 K, liquid	$(2.6 \pm 0.8) \times 10^{-3}$	[3]
	283-289 K, solid	$(3.8 \pm 1.0) \times 10^{-4}$	[3]
n-octanoic acid	290 K, liquid	$(2.1 \pm 0.3) \times 10^{-3}$	[3]
	287 K, solid	$(4.4 \pm 0.8) \times 10^{-4}$	[3]
Heptamethyl nonane	253 K, liquid	$(2.1 \pm 0.8) \times 10^{-3}$	[3]
	234 K, solid	$(2.6 \pm 0.9) \times 10^{-3}$	[3]
1-octanol	258 K, liquid	$(7.1 \pm 1.6) \times 10^{-3}$	[3]
	248 K, solid	$(5.2 \pm 2.0) \times 10^{-3}$	[3]

Table S2: Uptake coefficients for nitrate radical onto unsaturated organic substrates			
Substrate	Temperature and phase	γ	Source
Terminal C_{11} alkene monolayer	None specified	0.034	[4]
Oleic acid	302 K, liquid	0.21 (+0.79/-0.11)	[2]
	295 K, liquid	0.18 (+0.82/-0.06)	[2]
	288 K, liquid	0.16 (+0.84/-0.06)	[2]
	285 K, liquid	0.17 (+0.83/-0.09)	[2]
	283 K, solid	0.053 ± 0.011	[2]
	277 K, solid	0.051 ± 0.014	[2]
	268 K, solid	0.076 ± 0.026	[2]
Conjugated linoleic acid	298 K, liquid	0.37 (+0.63/-0.24)	[2]
	288 K, liquid	0.33 (+0.67/-0.21)	[2]
	278 K, liquid	0.62 (+0.38/-0.47)	[2]
	263 K, solid	0.08 ± 0.03	[2]
	273 K, liquid	$(7.9 \pm 0.2) \times 10^{-3}$	[3]
	253-263 K, solid	$(7.8 \pm 1.4) \times 10^{-3}$	[3]
Nonconjugated linoleic acid	298 K, liquid	0.29 (+0.71/-0.15)	[2]
	288 K, liquid	0.33 (+0.67/-0.20)	[2]
	278, liquid	0.41 (+0.59/-0.27)	[2]
	263, liquid	0.13 (+0.67/-0.05)	[3]
	288, liquid	$(1.5 \pm 0.2) \times 10^{-2}$	[3]
	248-263 K, solid	$(1.1 \pm 0.3) \times 10^{-2}$	[3]
1-octadecene	293 K, liquid	$(1.6 \pm 0.3) \times 10^{-3}$	[3]
	283 K, solid	$(1.4 \pm 0.1) \times 10^{-3}$	[3]
1-hexadecene	277 K, liquid	$(2.3 \pm 0.9) \times 10^{-3}$	[3]
	254-274 K, solid	$(1.8 \pm 0.3) \times 10^{-3}$	[3]
7-tetradecene	246 K, liquid	$(5.8 \pm 2.0) \times 10^{-3}$	[3]
	238 K, solid	$(5.2 \pm 2.0) \times 10^{-3}$	[3]

1. Knopf, D.A., J. Mak, S. Gross, and A.K Bertram (2006): Does atmospheric

processing of saturated hydrocarbon surfaces by NO_3 lead to volatilization?, *Geophys. Res. Lett., 33*, L17816, doi:10.1029/2006GL026884.

2. Gross, S., R. Iannone, S. Xiao, and A.K. Bertram (2009): Reactive uptake studies of NO_3 and N_2O_5 on alkenoic acid, alkanoate, and polyalcohol substrates to probe nighttime aerosol chemistry, *Phys. Chem. Chem. Phys., 11,* 7792-7803, doi: 10.1039/b904741g.

3. Moise, T., R.K. Talukdar, G.J. Frost, R.W. Fox, and Y. Rudich (2002): Reactive uptake of NO3 by liquid and frozen organics, *J. Geophys. Res., 107(D2),* 4014, doi:10.1029/2001JD000334.

4. Gross, S., and A.K. Bertram (2009): Products and kinetics of the reactions of an alkane monolayer and a terminal alkene monolayer with NO_3 radicals, *J. Geophys. Res., 114*, D02307, doi:10.1029/2008JD010987.

Table S3. Drop diameters and surface-area-to-volume ratios of aerosol bins

Bin number	Minimum diameter (μm)	Maximum diameter (μm)	Average radius (μm)	Average SA/vol (m)
a01	0.0390625	0.15625	0.048828	6.1440×10^{7}
a02	0.15625	0.625	0.195	1.54×10^{7}
a03	0.625	2.5	0.78	3.8×10^{6}
a04	2.5	10	3.1	9.7×10^{5}

Table S4. Vapor pressures for all products. Because of carbon number distribution and fragmentation, not all combinations of functional groups are possible for every carbon number. Shading indicates volatility: white: semivolatile in base model, light grey: nonvolatile in base model but semivolatile in sensitivity tests, dark grey: nonvolatile under all model conditions including sensitivity tests, brown: fully volatile under base model conditions.

# OH	2	2	3	3	2	2	1	1
# C=O	0	0	0	0	1	1	1	1
# COOH	1	1	1	1	1	1	0	1
# NO3	1	2	0	1	0	1	0	0
Carbons	Vapor pressures (Torr)							
3								1.08E-004
4								3.02E-004
5	9.97E-009	5.50E-011	9.83E-009	5.42E-011	2.10E-007	1.16E-009		3.86E-005
6	3.56E-009	1.97E-011	3.52E-009	1.94E-011	7.51E-008	4.14E-010		1.38E-005
7	1.27E-009	7.03E-012	1.26E-009	6.93E-012	2.69E-008	1.48E-010		4.94E-006
8	4.56E-010	2.51E-012	4.50E-010	2.48E-012	9.60E-009	5.30E-011		1.77E-006
9	1.63E-010	8.99E-013	1.61E-010	8.87E-013	3.43E-009	1.89E-011	2.60E-003	6.31E-007
10	5.83E-011	3.22E-013	5.74E-011	3.17E-013	1.23E-009	6.78E-012	9.45E-004	2.26E-007
11	2.08E-011	1.15E-013	2.06E-011	1.13E-013	4.39E-010	2.42E-012		
12	7.45E-012	4.11E-014	7.35E-012	4.06E-014	1.57E-010	8.67E-013		
13	2.67E-012	1.47E-014	2.63E-012	1.45E-014	5.62E-011	3.10E-013		
14	9.53E-013		9.40E-013		2.01E-011	1.11E-013		
15	3.41E-013		3.36E-013		7.18E-012	3.96E-014		
16	1.21E-013		1.20E-013		2.57E-012	1.42E-014		
17	4.36E-014		4.30E-014		9.19E-013			
18	1.56E-014		1.54E-014		3.29E-013			
19					1.18E-013			
20					4.20E-014			

Appendix: Representative WRF/Chem namelist file.

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run_hours                = 0,
run_minutes              = 0,
run_seconds              = 0,
start_year               = 2008,
start_month              = 05,
start_day                = 1,
start_hour               = 00,
start_minute             = 00,
start_second             = 00,
end_year                 = 2008,
end_month                = 05,
end_day                  = 31,
end_hour                 = 00,
end_minute               = 00,
end_second               = 00,
interval_seconds         = 21600,
input_from_file          = .true.,
history_interval         = 60,
frames_per_outfile       = 24,
restart                  = .false.,
restart_interval         = 1440,
auxinput5_interval_m     = 60,
io_form_history          = 2,
io_form_restart          = 2,
io_form_input            = 2,
io_form_boundary         = 2,
io_form_auxinput4        = 2,
io_form_auxinput5        = 2,
debug_level              = 0,
/

 &domains
time_step                = 30,
time_step_fract_num      = 0,
time_step_fract_den      = 1,
max_dom                  = 1,
s_we                     = 1,
e_we                     = 90,
s_sn                     = 1,
e_sn                     = 180,
s_vert                   = 1,
e_vert                   = 28,
p_top_requested                  = 10000,
num_metgrid_levels               = 30,
num_metgrid_soil_levels          = 4,
dx                       = 12000,
dy                       = 12000,
grid_id                  = 1,
parent_id                = 0,
i_parent_start           = 1,
j_parent_start           = 1,
parent_grid_ratio        = 1,
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/

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mp_physics               = 3,
ra_lw_physics            = 1,
ra_sw_physics            = 1,
radt                     = 30,
sf_sfclay_physics        = 1,
sf_surface_physics       = 3,
bl_pbl_physics           = 1,
bldt                     = 0,
cu_physics               = 1,
cudt                     = 5,
isfflx                   = 1,
ifsnow                   = 0,
icloud                   = 1,
surface_input_source     = 1,
num_soil_layers          = 4,
sf_urban_physics                 = 0,
maxiens                  = 1,
maxens                   = 3,
maxens2                  = 3,
maxens3                  = 16,
ensdim                   = 144,
/

&fdda
/

 &dynamics
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 km_opt                        = 4,
 diff_6th_opt                  = 0,      0,      0,
 diff_6th_factor               = 0.12,   0.12,   0.12,
 base_temp                     = 290.
 damp_opt                      = 0,
 zdamp                         = 5000.,  5000.,  5000.,
 dampcoef                      = 0.2,    0.2,    0.2
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 kvdif                         = 0,      0,      0,
 non_hydrostatic               = .true., .true., .true.,
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 scalar_adv_opt                = 2,      1,      1,
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spec_zone                = 1,
relax_zone               = 4,
specified                = .true.,
periodic_x               = .false.,
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symmetric_xe            = .false.,
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open_ye                 = .false.,
nested                  = .false.,
/

&grib2
/

&chem
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 bioemdt                         = 30,
 photdt                          = 30,
 chemdt                          = 2.,
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 io_style_emissions              = 1,
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 emiss_opt                       = 3,
 chem_in_opt                     = 0,
 phot_opt                        = 3,
 drydep_opt                      = 1,
 bio_emiss_opt                   = 1,
 dust_opt                        = 0,
 dmsemis_opt                     = 0,
 seas_opt                        = 0,
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 gas_ic_opt                      = 1,
 aer_bc_opt                      = 1,
 aer_ic_opt                      = 1,
aer_op_opt                       =2,
gaschem_onoff                    = 1,
 aerchem_onoff                   = 1,
 wetscav_onoff                   = 0,
 cldchem_onoff                   = 0,
 vertmix_onoff                   = 1,
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 /


&namelist_quilt
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nio_groups               = 1,
/
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