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

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This supplemental information shows the experimental data used to determine average NO_3 uptake onto saturated (Fig. S1) and unsaturated (Fig. S2) organic in aerosol, the surface area of each aerosol size bin (Fig. S3), and a representative WRF/Chem namelist file (Appendix). All western US and Pacific Northwest monthly and daily OA source and sink spatial maps are available upon request (fry@reed.edu).

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}

Appendix: Representative WRF/Chem namelist file.

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&time_control
run_days                 = 31,
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,
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```
parent_grid_ratio       = 1,
parent_time_step_ratio   = 1,
feedback              = 1,
smooth_option          = 0,
/

&physics
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
 w_damping                  = 0,
 diff_opt                 = 1,
 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
 khdif                    = 0,      0,      0,
 kvdif                    = 0,      0,      0,
 non_hydrostatic              = .true., .true., .true.,
 moist_adv_opt              = 2,      1,      1,
 scalar_adv_opt             = 2,      1,      1,
 /


&bdy_control
spec_bdy_width         = 5,
spec_zone            = 1,
relax_zone           = 4,
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specified             = .true.,
periodic_x            = .false.,
symmetric_xs          = .false.,
symmetric_xe          = .false.,
open_xs               = .false.,
open_xe               = .false.,
periodic_y            = .false.,
symmetric_ys          = .false.,
symmetric_ye          = .false.,
open_ys               = .false.,
open_ye               = .false.,
nested                = .false.,
/

&grib2
/

&chem
 kemit                          = 19,
 chem_opt                       = 7,
 bioemdt                        = 30,
 photdt                         = 30,
 chemdt                         = 2.,
 frames_per_emissfile           = 12,
 io_style_emissions             = 1,
 emiss_inpt_opt                 = 102,
 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,
 gas_bc_opt                     = 1,
 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,
 chem_conv_tr                   = 1,
 biomass_burn_opt               = 0,
 plumerisefire_frq              = 30,
 aer_ra_feedback                = 1,
 have_bcs_chem                  = .false.,

 /


&namelist_quilt
nio_tasks_per_group     = 0,
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nio_groups              = 1,
/
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