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Supplement of

MultilayerPy (v1.0): a Python-based framework for building, running and optimising kinetic multi-layer models of aerosols and films

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S1. Parameter correlation

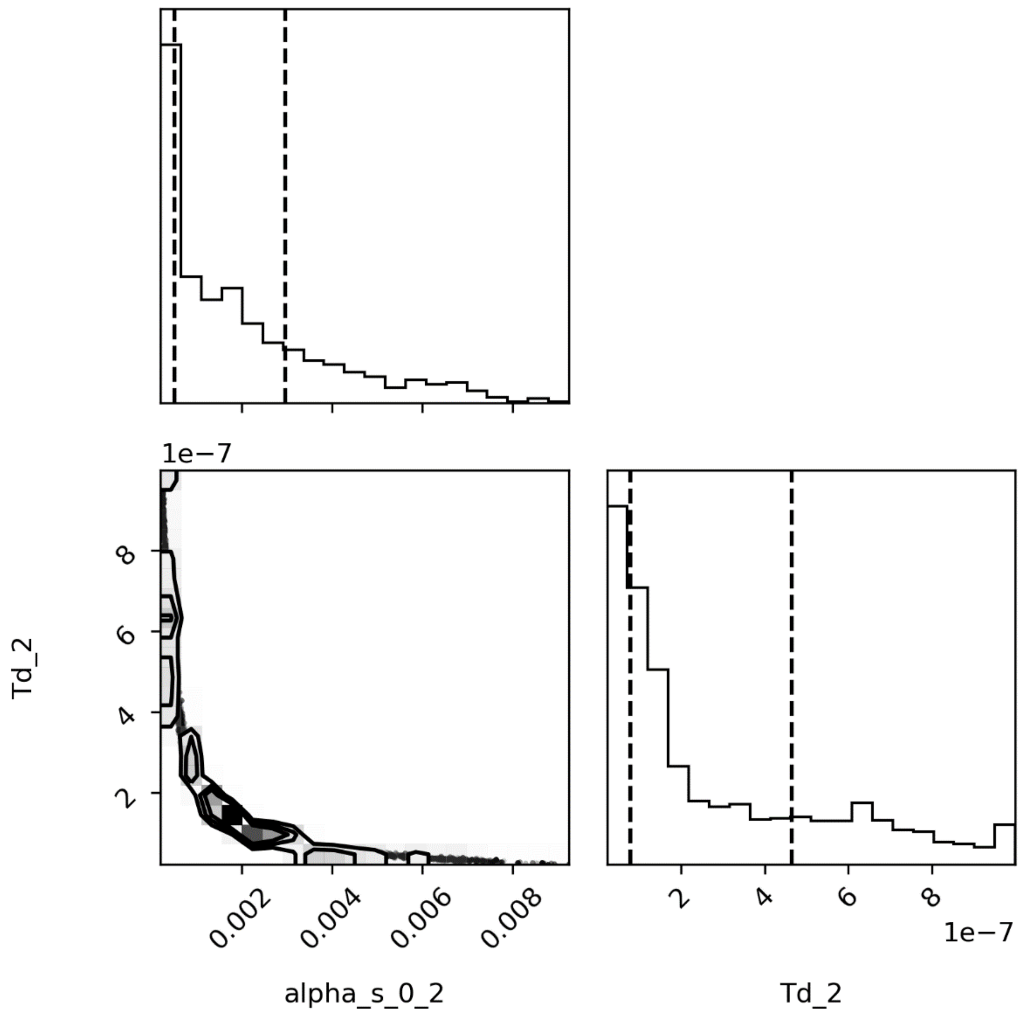

Figure S1. A corner plot derived from the MCMC sampling procedure simultaneously varying the surface accommodation coefficient of ozone (alpha_s_0_2, component 2) and the surface desorption lifetime of ozone (Td_2, component 2) described in the main text. Inter-quartile ranges are denoted by dashed lines.

There is a range of possible parameter combinations consistent with the experimental data (Fig. S1). The lack of a gaussian "blob" in the corner plot indicates that these two parameters are highly correlated and that one (or ideally, both) should be constrained.

S2. Reaction scheme and table of parameters used for KM-SUB and KM-GAP case study 1

The reaction scheme used for both KM-SUB and KM-GAP models is as follows (component numbers employed in MultilayerPy are in square brackets):

[1]Oleic acid + [2]Ozone → [3]Non-volatile products + [4]Nonanal

Parameter name	Description	Parameter value [bounds]
Db_1	Bulk diffusion coefficient of oleic acid (component 1)	10^{-10} cm^2 s^{-1}
Db_2	Bulk diffusion coefficient of ozone (component 2)	10^{-5} cm^2 s^{-1}
Db_3	Bulk diffusion coefficient of products (component 3)	10^{-10} cm^2 s^{-1}
T	Temperature	298 K
delta_1	Molecular diameter of oleic acid (component 1)	0.8×10^{-7} cm
delta_2	Molecular diameter of ozone (component 2)	0.4×10^{-7} cm
delta_3	Molecular diameter of products (component 3)	0.4×10^{-7} cm
k_1_2	Bulk reaction rate coefficient for oleic acid reacting with ozone	1.7×10^{-15} cm^3 s^{-1}
k_1_2_surf	Surface reaction rate coefficient for oleic acid reacting with ozone	6×10^{-12} cm^2 s^{-1}
Xgs_2	Near-surface gas concentration for ozone (component 2)	7×10^{13} cm^{-3}
Td_2	Surface desorption lifetime of ozone (component 2)	0.02 s
Td_4 (KM-GAP)*	Surface desorption lifetime of nonanal (component 4)	0.1 s [10^{-4} – 10^{-1}]
H_2	Henry's law coefficient for ozone (component 2)	4.8×10^{-4} mol cm^{-3} atm^{-1}
w_2	Mean thermal velocity of ozone in the gas phase	3.6×10^{4} cm s^{-1}
alpha_s_0_2**	Surface accommodation coefficient of ozone on a clear surface	4.2×10^{-4} [10^{-4} – 10^{-1}]
p_2	Vapour pressure of ozone (component 2)	5.7×10^{6} Pa
p_4***	Vapour pressure of nonanal (component 4)	10 Pa

Table S1. Parameters used to run the KM-SUB and KM-GAP models presented in the main text. *The surface desorption lifetime of all non-volatile components was set to a very large value (10^6 s) in the KM-GAP model. **The optimised value from the KM-GAP model was 10^{-3}. ***vapour pressures of all other non-volatile components set to 0 in the KM-GAP model.