Supplementary of

Modeling new particle formation in the remote marine atmosphere using a nitric acid-based nucleation scheme in WRF-Chem

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1. Model

Bin	Lower diameter (nm)	Upper diameter (nm)
1	1.00	2.15
2	2.15	4.64
3	4.64	10.00
4	10.00	21.50
5	21.50	46.40
6	46.40	100.00
7	100.00	215.00
8	215.00	464.00
9	464.00	1000.00
10	1000.00	2150.00
11	2150.00	4640.00
12	4640.00	10000.00

Table S1 Particle size distribution in MOSAIC using a 12-bin section approach (Lupascu et al., 2015)

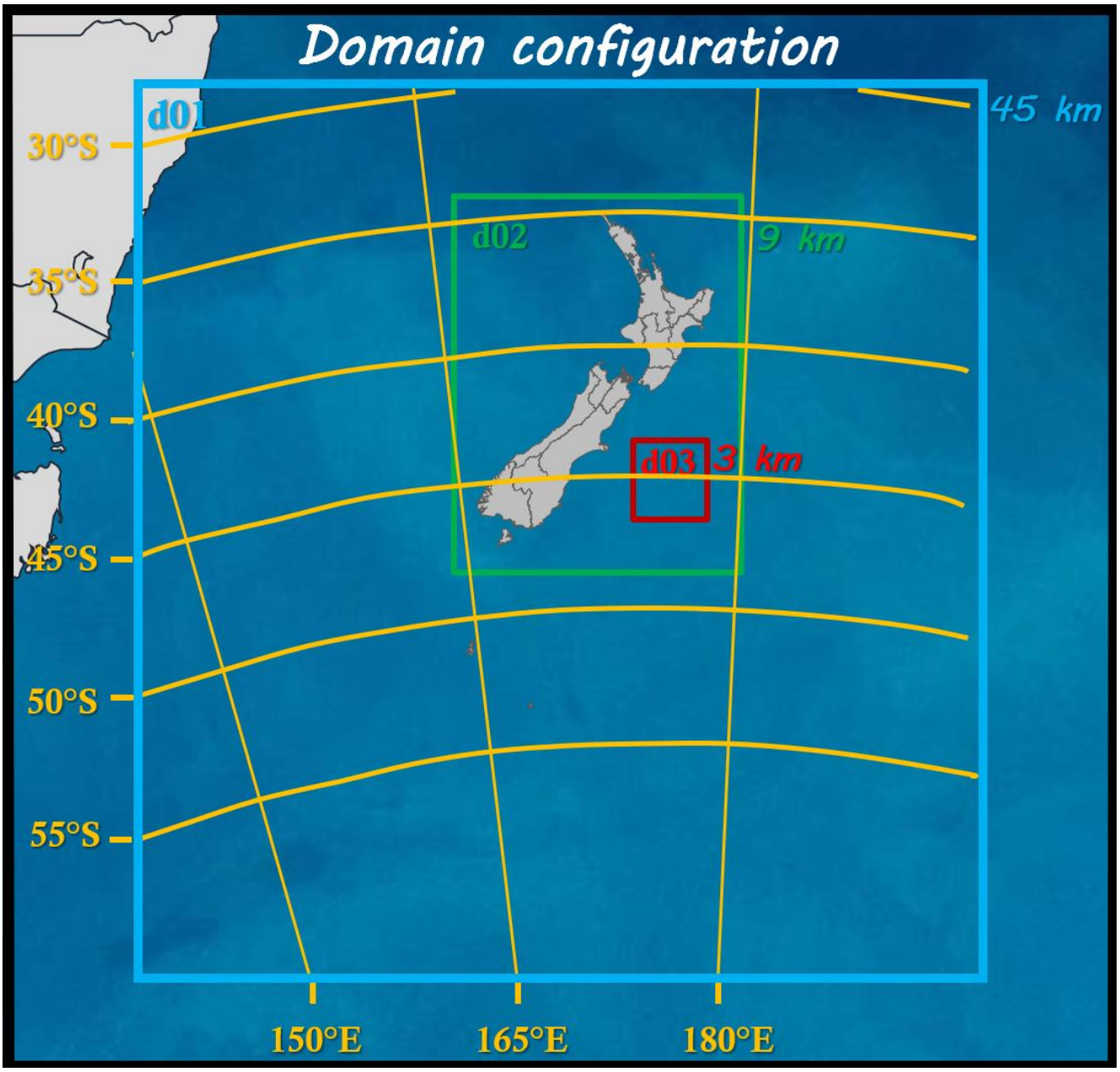


Figure S1 extend of WRF-Chem's three domains with horizontal resolution of 45 (d01), 9 (d02) and 3 km (d03).

2. Analysis of the aerosol size distribution

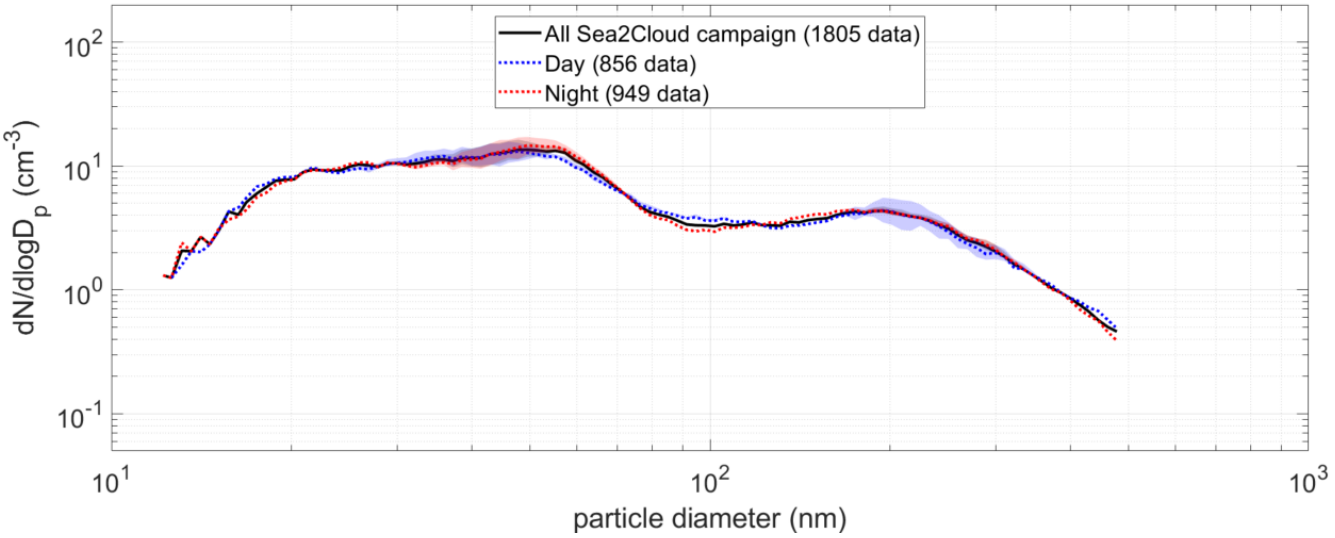


Figure S2 Median aerosol size distribution measured with the SMPS in clean ambient marine air masses during the Sea2Cloud campaign, classified by daytime (red dotted line), nighttime (blue dotted line), and the 24-hour median (black dotted line).

3. Detection and characterization of nucleation events

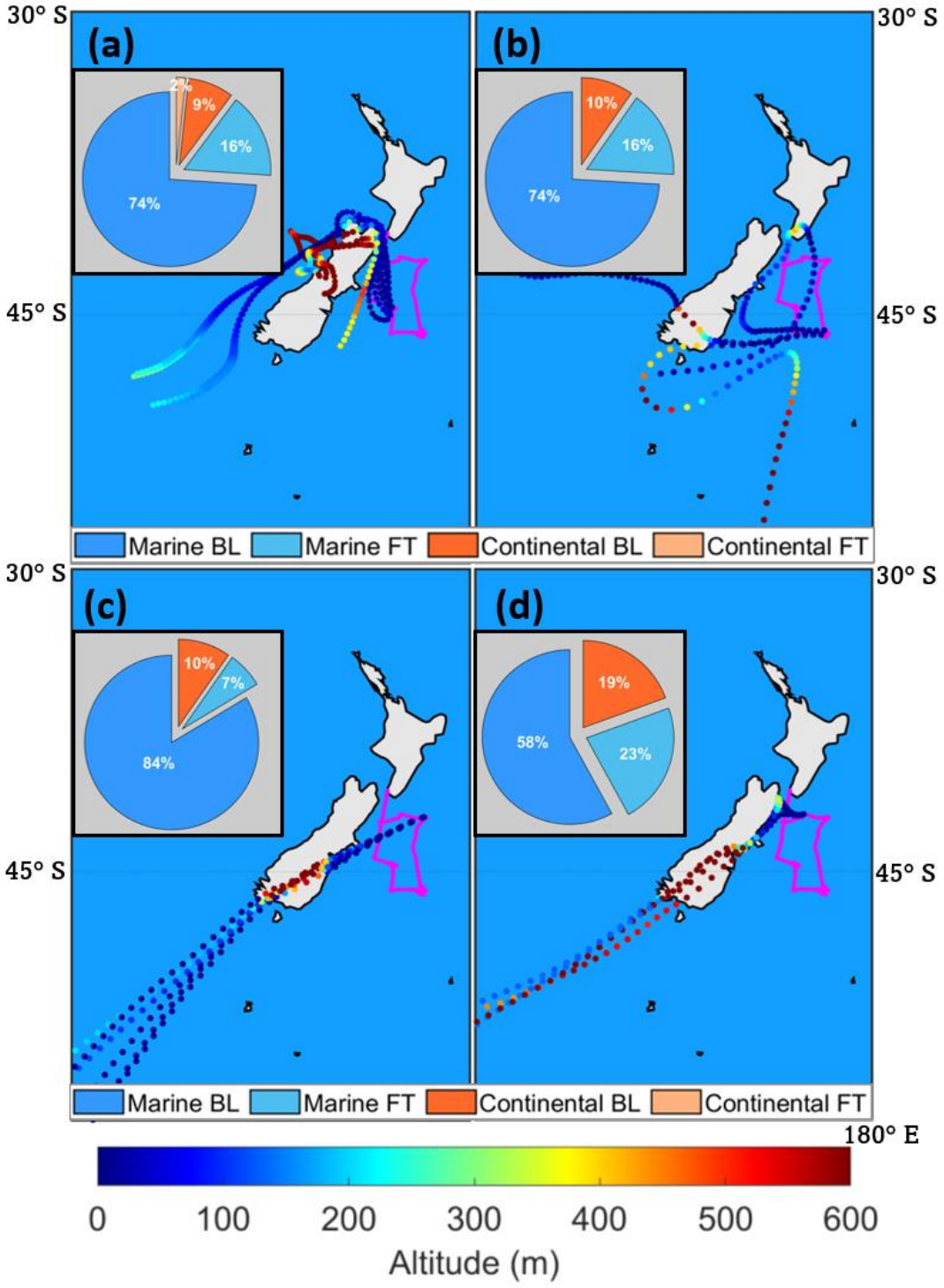


Figure S3 Air mass back-trajectories calculated using the HYSPLIT model over the 72 hours preceding the position of the *R/V Tangaroa* (in rose) on (a) March 19, 2020 (09:00 – 16:00 UTC), (b) March 22, 2020 (06:00 – 08:00 UTC), (c) March 24, 2020 (01:00 – 06:00 UTC), and (d) March 24, 2020 (16:00 – 19:00 UTC). The color scale represents the altitude (in meters) of the air masses along their trajectory. Pie charts depicts the percentage of hours spent by air masses within the boundary layer (BL) or the free troposphere (FT), whether in a marine or continental atmosphere.

4. Dependence of simulated particle concentrations to HNO_3 levels in the marine boundary layer

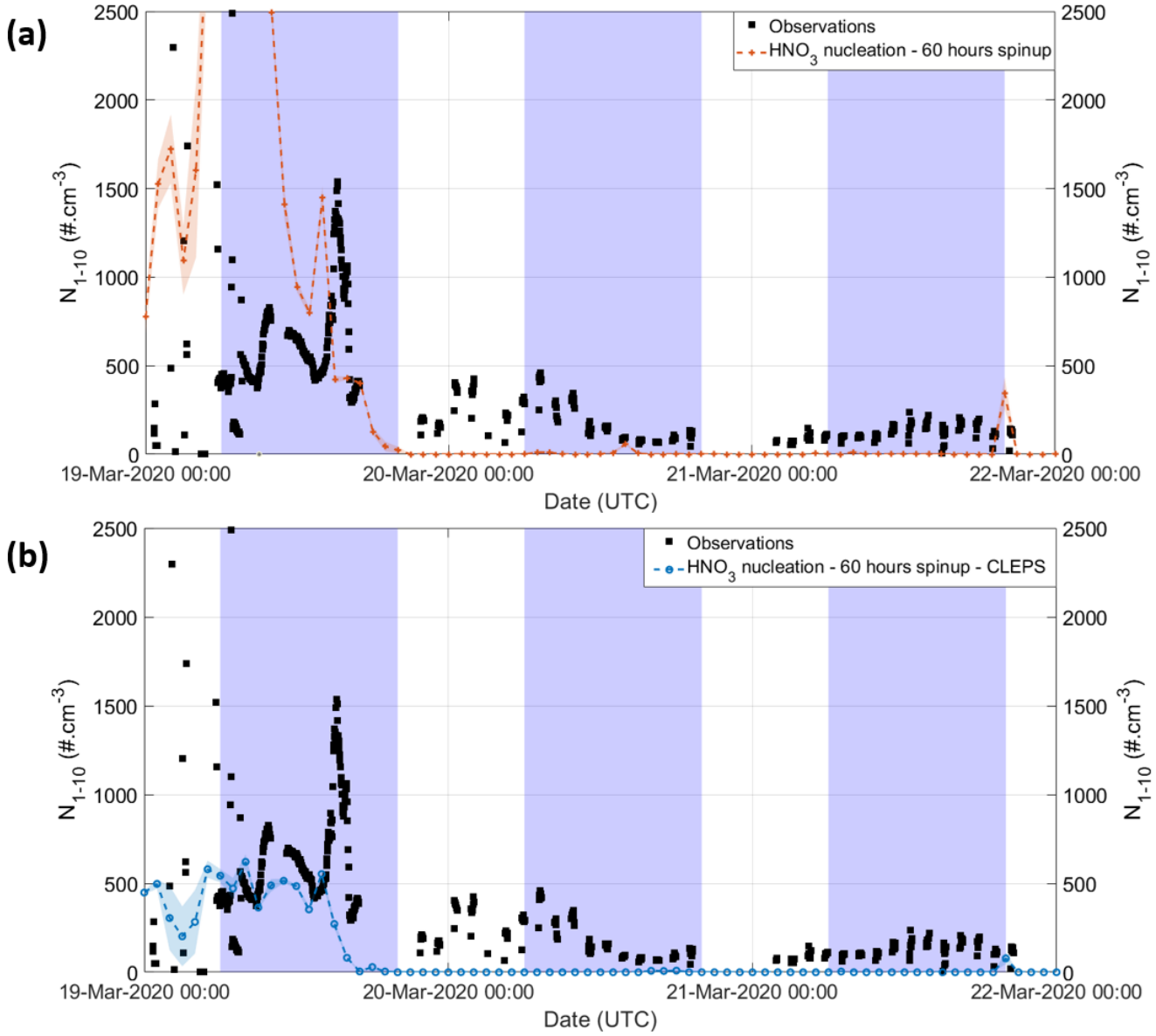


Figure S4 Time series of discrete observations (left-axis) and simulated hourly (right-axis) particle number concentrations using the new nitric acid nucleation mechanism (Equation 1). Panel (a) shows results using a spin-up length of 60 hours, while panel (b) shows results from the CLEPS experimental conditions, where nucleation is triggered only when nitric acid concentrations are <~2.5 x 10^7 molec.cm^{-3}, (i.e., in the range of validity of the parameterization determined from our experimental conditions) with the same 60-hour spin-up. Blue patches depict night-time periods, and shaded boundaries around modeled concentrations represent their standard deviation along the ship's path.

5. Simulation of N_{1-10} with the new nitric acid-based nucleation mechanism

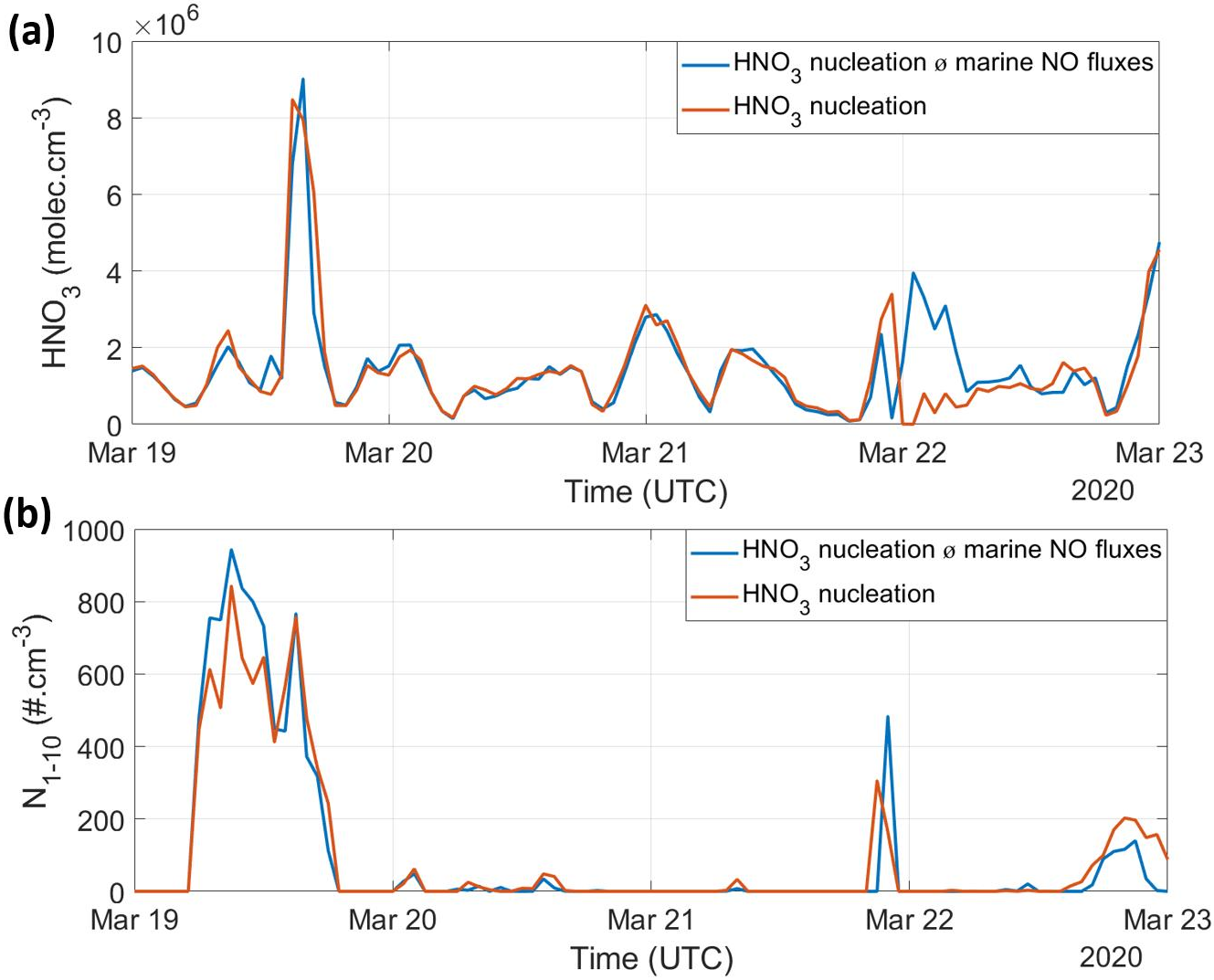


Figure S5 Time series of simulated hourly (a) HNO_3 concentrations and (b) particle number concentrations between 1 and 10 nm using the new nitric acid nucleation mechanism presented in Salignat et al. (submitted) with (*HNO_3 nucleation*) or without (*HNO_3 nucleation Ø marine NO fluxes*) seawater biogenic NO emissions.

6. Preliminary assessment of new particle formation in the upper atmosphere

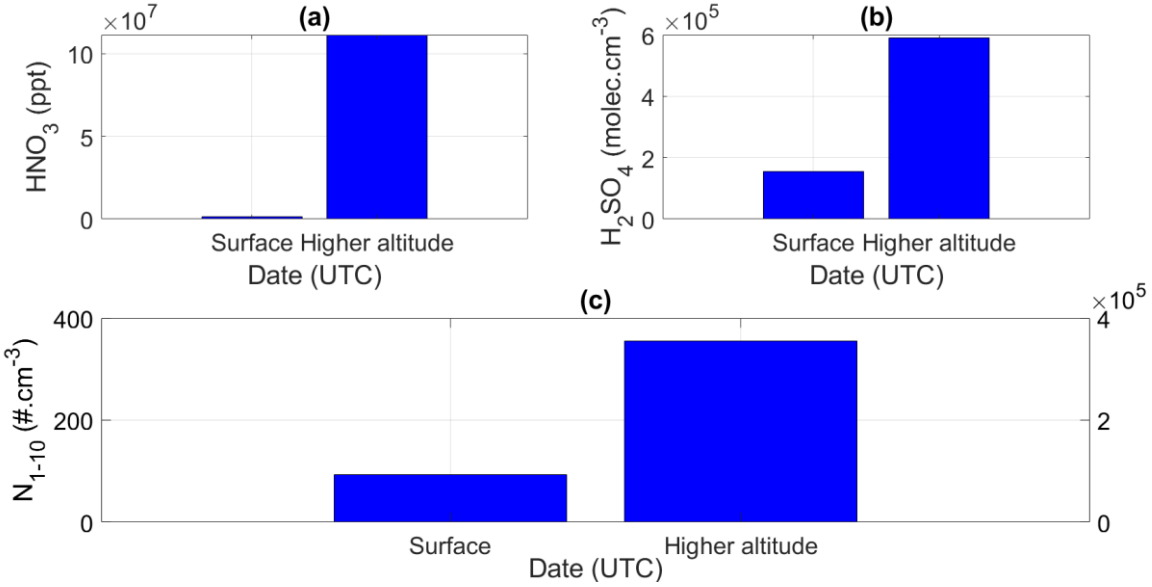


Figure S6 Mean concentrations of simulated (a) HNO_3 (ppt), (b) H_2SO_4 (molec.cm^{-3}), and (c) $N_{1\text{-}10}$ (#.cm^{-3}) along the Sea2Cloud trajectory. Panels (a, b, and c) compare concentrations between the lower (surface) and upper (higher altitude) troposphere. Note that the scales on (c) vary depending on the axis.