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Oxidation-driven acceleration of NPF-to-CCN conversion under polluted atmosphere: evidence from mountain-top observations in Yangtze River Delta

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S1. Observation-based model

In this study, a box model (the Framework for 0-dimensional Atmospheric Modeling (F0AM)) and the main chemical mechanism (MCM v3.3.1) were applied to simulate the formation of gaseous nitric acid during the NPF growth process at the observation site in the spring season. The F0AM model is a photochemical box model widely used for simulating atmospheric chemistry. The atmospheric chemistry in this study is based on MCM v3.3.1 (http://mcm.leeds.ac.uk/MCM/), which includes approximately 6,000 species and 17,000 reactions. In this study, based on the observed species, the model utilized 3417 species and 10926 reactions. Observed data were input into the F0AM model, including NO, NO_2, O_3, SO_2, nitrates, 67 VOC species, relative humidity, temperature, atmospheric pressure, particulate matter surface area concentration, boundary layer height, j (O_1D), j (NO_2), j (HONO), etc. Please note that we did not consider horizontal and vertical transport in the atmospheric box model. Therefore, to prevent the accumulation of long-lived oxidation products, a 24 hour first-order dilution rate was adopted (Zhao et al., 2020). For more details on the model settings, please refer to our previous studies (Liu et al., 2021; Han et al., 2023).

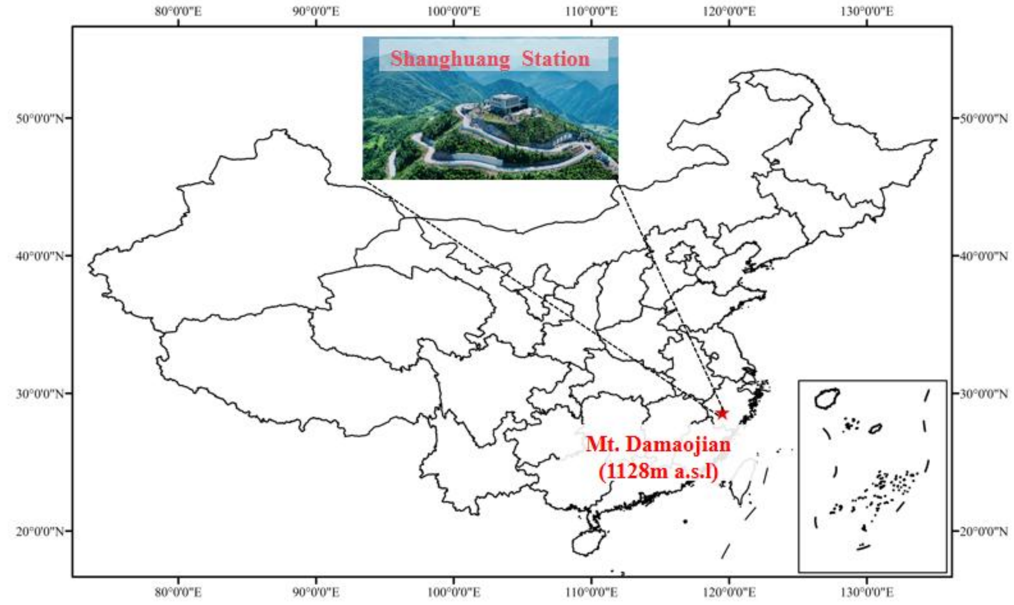

Figure S1: Location of the Shanghuang station.

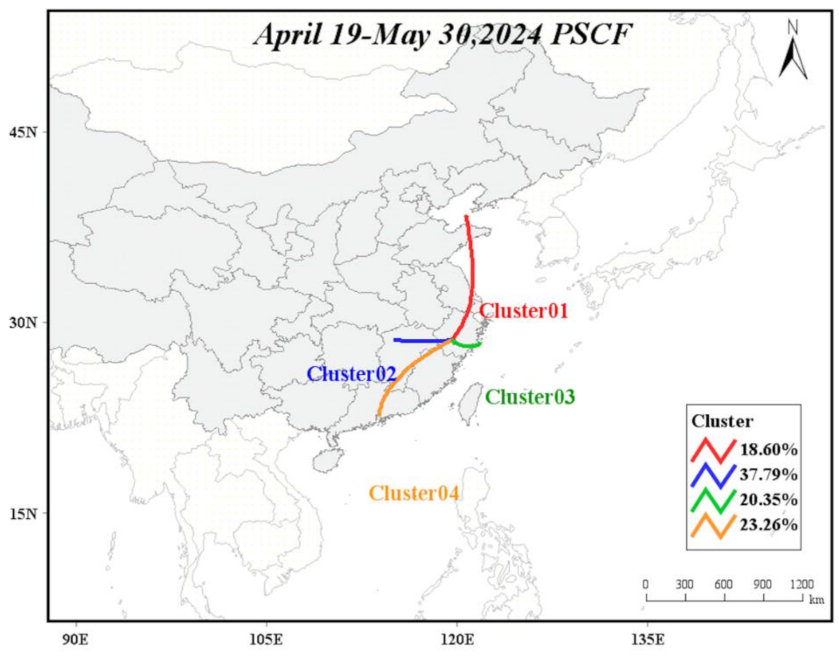

Figure S2: A 72-hour backward trajectory analysis was performed on the air masses throughout the entire observation period, resulting in four different classifications of air masses based on their sources.

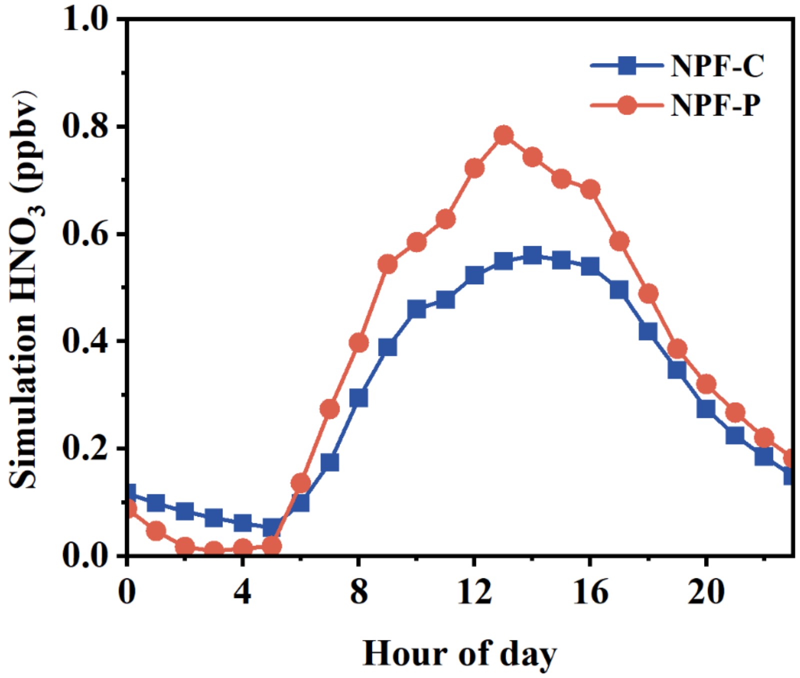

Figure S3: Daily variations in gaseous nitric acid (HNO_3) concentrations corresponding to two types of NPF events, based on F0AM simulation data. Red represents NPF-P events, and blue represents NPF-C events.

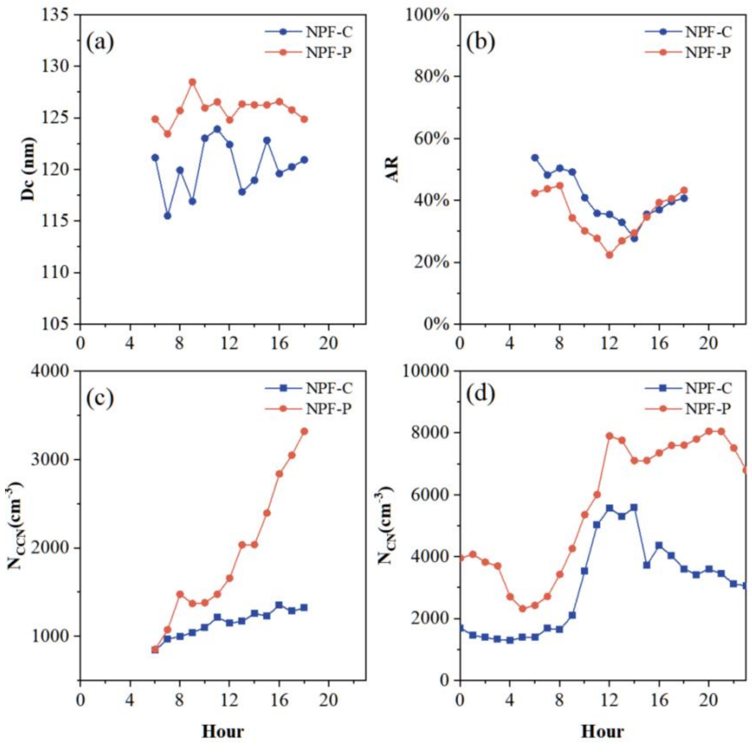

Figure S4: The diurnal variation of critical activation diameter (D_a), activation ratio (AR), the number of cloud condensation nuclei (N_{CCN}) and total particle number concentration (N_{CN}) in NPF-C and NPF-P events. The blue line denotes to NPF-C events and red line denotes to NPF-P events.

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