SUPPORTING INFORMATION

Cluster Dynamics-based Parameterization for Sulfuric Acid-Dimethylamine Nucleation: Comparison and Selection through Box- and Three-Dimensional-Modeling

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Totally 11 Figures and 2 Tables

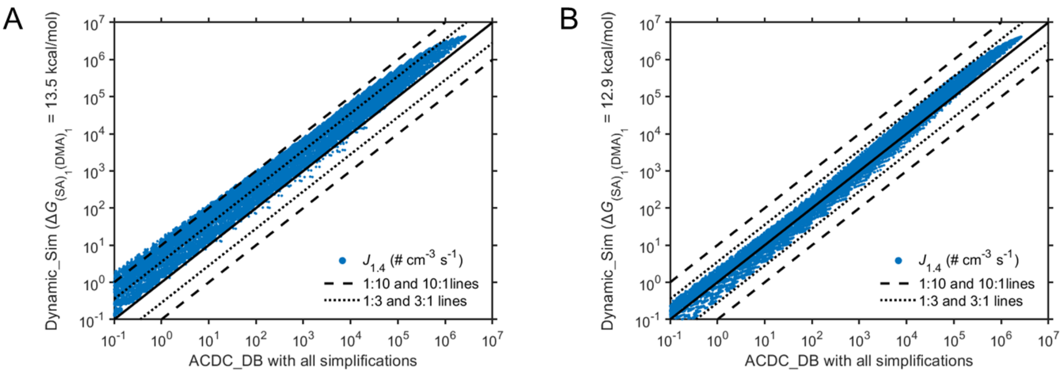

Figure S1. Comparison of $J_{1.4}$ predictions between ACDC_DB with all simplifications and Dynamic_Sim with different ΔG for initial $(SA)_1(DMA)_1$ cluster. A: ΔG = 13.5 kcal/mol; B: ΔG = 12.9 kcal/mol (Ning et al. 2024). Solid dots represent simulated $J_{1.4}$ values, solid lines indicate a 1:1 line, dotted lines correspond to 1:3 and 3:1 lines, and dashed lines represent 1:10 and 10:1 lines.

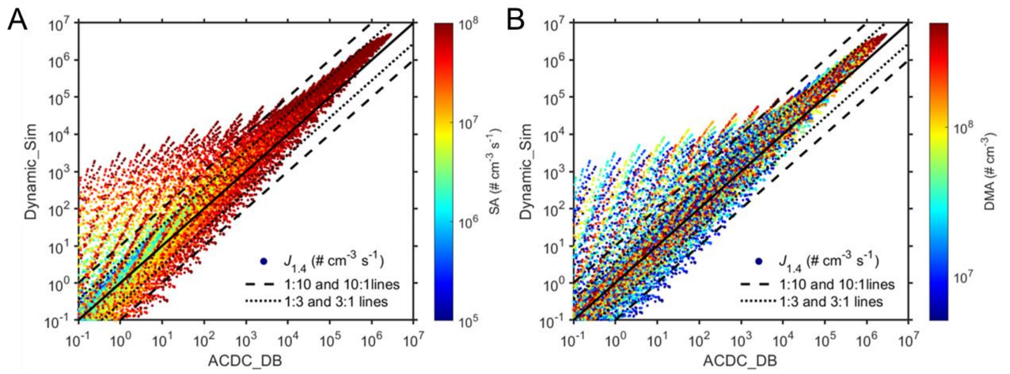

Figure S2. Comparison of $J_{1.4}$ predictions between ACDC_DB and Dynamic_Sim correlated with [SA] variation (A) and [DMA] variation (B). Solid dots represent simulated $J_{1.4}$ values, solid lines indicate a 1:1 line, dotted lines correspond to 1:3 and 3:1 lines, and dashed lines represent 1:10 and 10:1 lines.

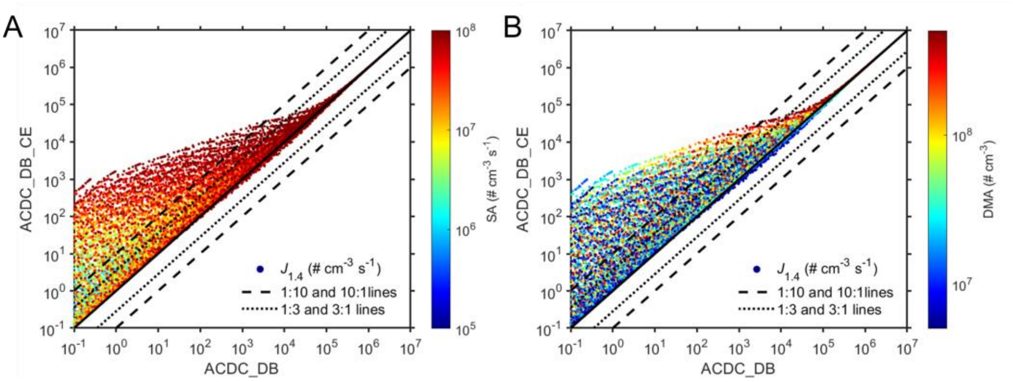

Figure S3. Same as Figure S2 but for ACDC_DB_CE.

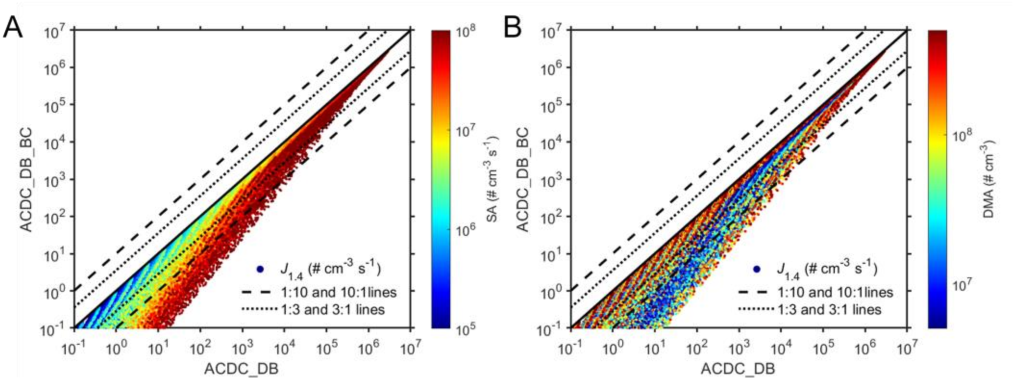

Figure S4. Same as Figure S2 but for ACDC_DB_BC.

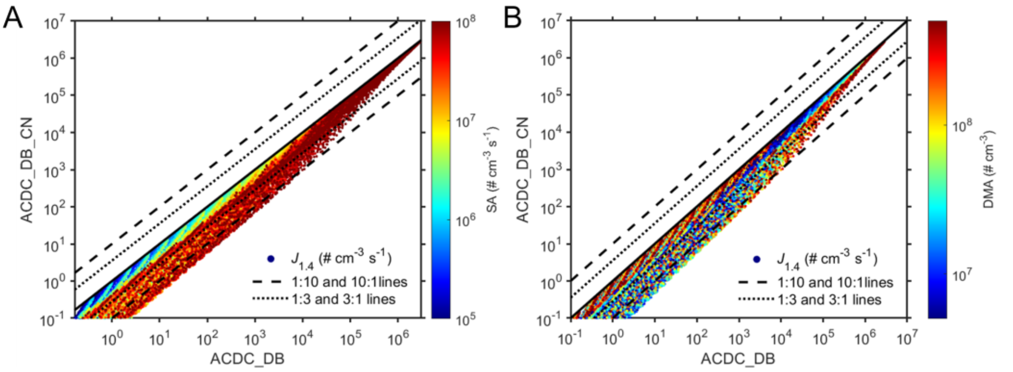

Figure S5. Same as Figure S2 but for ACDC_DB_CN.

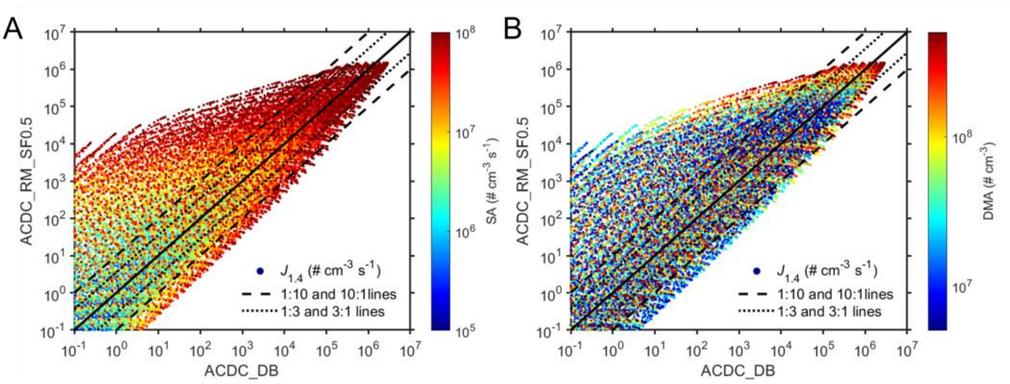

Figure S6. Same as Figure S2 but for ACDC_RM_SF0.5.

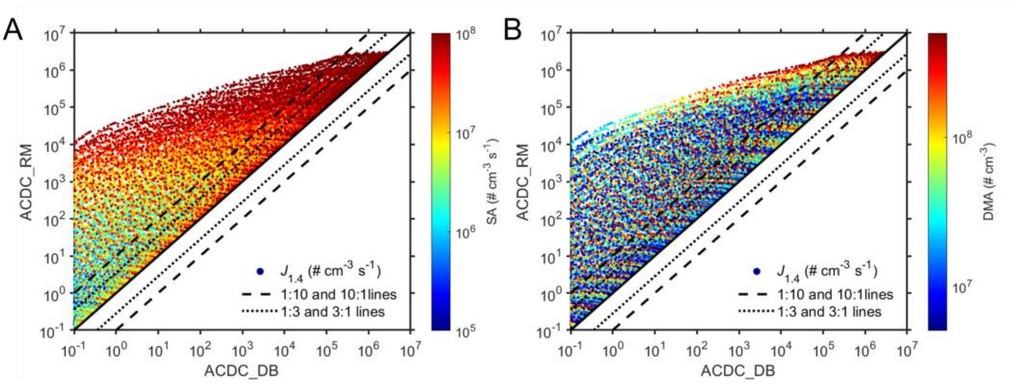

Figure S7. Same as Figure S2 but for ACDC_RM.

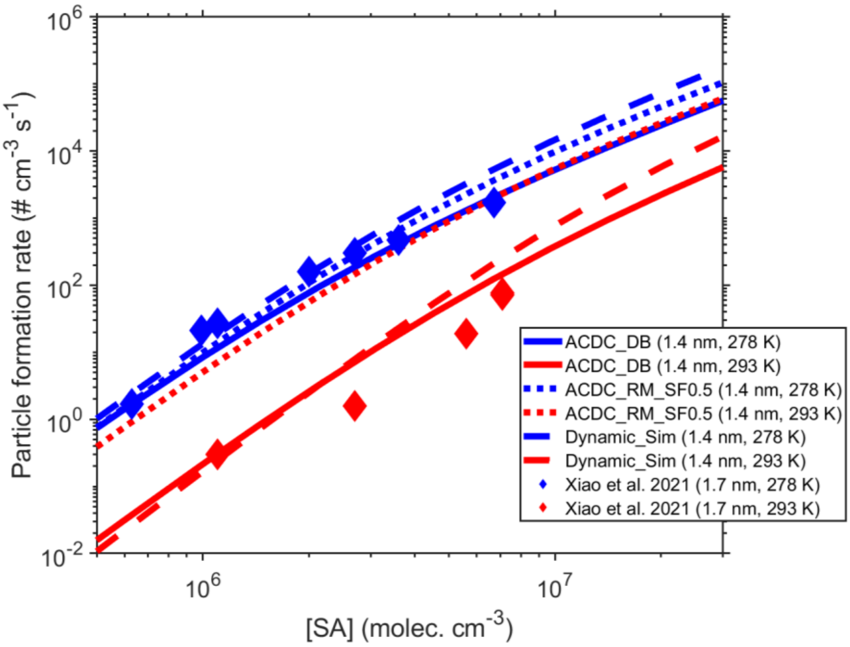

Figure S8. Comparison of modeled particle formation rates with measurements from CLOUD chamber experiments conducted by Xiao et al. 2021. Blue lines or diamonds represent particle formation rates at 278 K, while red ones represent those at 293 K; solid, dotted, and dashed lines denote the simulated results of ACDC_DB, ACDC_RM_SF0.5, and Dynamic_Sim, respectively. The simulations were conducted following the experimental conditions of Xiao et al. 2021, with specific conditions provided in their Table S1 and Table S2. It is noteworthy that Xiao et al. 2021 reported particle formation rates at 1.7 nm, whereas our simulations are at 1.4 nm. This discrepancy may lead to a slight overestimation of the simulated particle formation rates for simulations compared to the experiments. However, in the experiments, ~1 ppbv NH_3 was involved besides DMA during nucleation, which might enhance nucleation rates somewhat even through DMA is the dominant enhancing agent for SA-driven nucleation. Therefore, the two effects could partly offset each other, allowing for a direct comparison of particle formation rates between simulations and measurements.

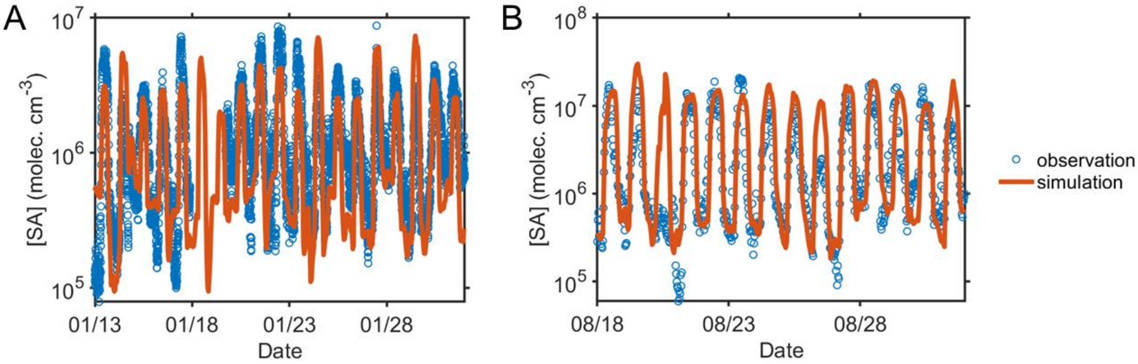

Figure S9. Comparison of simulated and observed SA concentrations. A for January and B for August 2019.

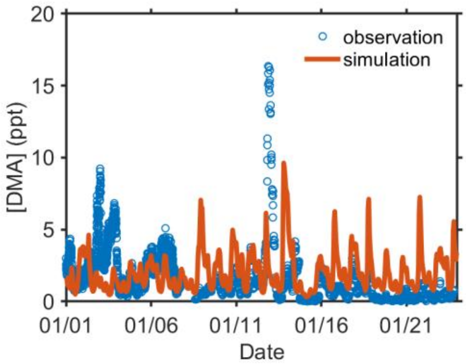

Figure S10. Comparison of simulated and observed DMA concentrations in January 2019. Only data for winter month (January 2019) is available.

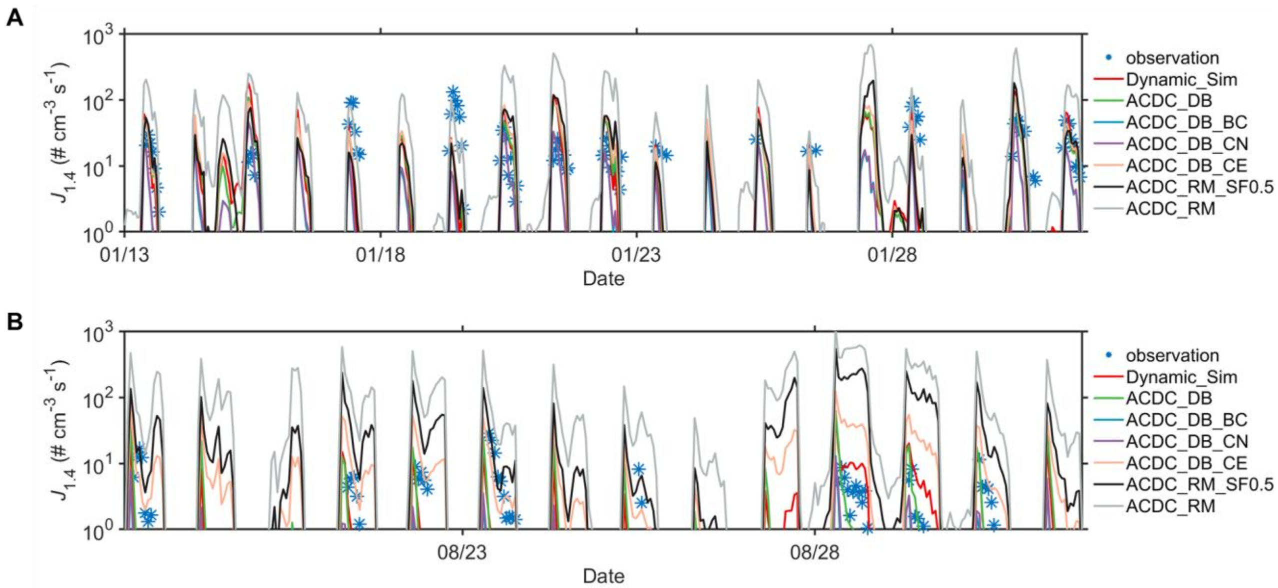

Figure S11. Comparison of simulated particle formation rates with those derived from field measurements during (A) January 13, 2019, to January 31, 2019, and (B) August 18, 2019, to August 31, 2019, in Beijing.

Table S1. The ranges, total numbers and values at each point for the input parameters in deriving look-up tables

	Range	Number of points	Values at each point
T (K)	250 – 320	15	$250 + 5 \times i$, $i = 1,15$
CS (s^{-1})	$5 \times 10^{-4} – 5 \times 10^{-1}$	16	$5 \times 10^{-4} \times 10^{0.2 \times i}$, $i = 1,16$
[SA] (# cm^{-3})	$1 \times 10^{5} – 1 \times 10^{8}$	16	$1 \times 10^{5} \times 10^{0.2 \times i}$, $l = 1,16$
[DMA] (# cm^{-3})	$5 \times 10^{6} – 1 \times 10^{8}$	11	$5 \times 10^{6} \times 10^{0.2 \times i}$, $i = 1,11$

Table S2. Comparison of simulated and observed concentrations of the nucleating precursors.

Precursor	Time period	Site	Simulation	Observation	Bias	NMB
SA (#/cm^3)	2019.01.13-2019.01.31	Beijing	1.35×10^{6}	1.47×10^{6}	1.20×10^{5}	-10.80%
	2019.08.18-2019.08.31		5.74×10^{6}	3.51×10^{6}	2.23×10^{6}	14.32%
DMA (pptv)	2019.01.01-2019.01.31	Beijing	1.96	1.98	-0.02	-10.96%

REFERENCES

Xiao, M., Hoyle, C. R., Dada, L., Stolzenburg, D., Kürten, A., Wang, M., Lamkaddam, H., Garmash, O., Mentler, B., Molteni, U., Baccarini, A., Simon, M., He, X.-C., Lehtipalo, K., Ahonen, L. R., Baalbaki, R., Bauer, P. S., Beck, L., Bell, D., Bianchi, F., Brilke, S., Chen, D., Chiu, R., Dias, A., Duplissy, J., Finkenzeller, H., Gordon, H., Hofbauer, V., Kim, C., Koenig, T. K., Lampilahti, J., Lee, C. P., Li, Z., Mai, H., Makhmutov, V., Manninen, H. E., Marten, R., Mathot, S., Mauldin, R. L., Nie, W., Onnela, A., Partoll, E., Petäjä, T., Pfeifer, J., Pospisilova, V., Quéléver, L. L. J., Rissanen, M., Schobesberger, S., Schuchmann, S., Stozhkov, Y., Tauber, C., Tham, Y. J., Tomé, A., Vazquez-Pufleau, M., Wagner, A. C., Wagner, R., Wang, Y., Weitz, L., Wimmer, D., Wu, Y., Yan, C., Ye, P., Ye, Q., Zha, Q., Zhou, X., Amorim, A., Carslaw, K., Curtius, J., Hansel, A., Volkamer, R., Winkler, P. M., Flagan, R. C., Kulmala, M., Worsnop, D. R., Kirkby, J., Donahue, N. M., Baltensperger, U., El Haddad, I., and Dommen, J.: The driving factors of new particle formation and growth in the polluted boundary layer, Atmospheric Chemistry and Physics, 21, 14275-14291, 10.5194/acp-21-14275-2021, 2021.