We are very grateful to the evaluations from the reviewers, which have allowed us to clarify and improve the manuscript. Below we addressed the reviewer comments, with the reviewer comments in black and our response in blue. The changes in the revised manuscript are indicated in italics and line number that we refer to is the tracked version (All Markup) of the revised manuscript.

Reply for the referee #2 - Mao et al.

General comments: Particle number concentrations, as computed by the available parametrization scheme for nucleation within the CMAQ model, did not agree well with observations (in China), and the authors have incorporated few other schemes and conducted simulations. Along with few individual schemes, numerical experiments combining few schemes together, have also been carried out. The Paper suggests enhanced capability of the model with the implemented schemes.

Overall manuscript is a significant advancement and the discussions are clear. The manuscript is recommended for publication in GMD. The following comments are provided for authors to consider during the revision process.

General Response: We greatly appreciate the referee for their time and efforts devoted to the review of our submission. We realize that most of the comments arise from the unclear in the content description. We will present these details in the following responses.

Specific comments and responses:

1.81: "WRF-Chem proves that HIO₃ nucleation is the main way in future". This is not very clear. Review and reframe this discussion.

Response: We apologize for any inaccuracies in the expressions. We have revised the sentence in Line 81 to "By coupling all the different forms of nucleation parameterization schemes discussed above, the E3SM model indicates that H2SO4-dimethylamine nucleation dominates number concentration in 1 km height (Zhao et al., 2024). Based on this result, the Weather Research and Forecasting model coupled with chemistry (WRF-chem), established the same nucleation parameterization schemes, proves that HIO3 nucleation is the main nucleated way in the future (Ning et al., 2024)."

1.97-98: The approach SumBTD and SumID are not clear to me. I did not find much description of these approaches. How do you combine several options of nucleation together? How do you decide which of the options should be combined like in case of BTD or in case of ID, instead of other possible combinations?

Response: Thanks for your comment. To clarify this, we have revised the sentence in Line 205 to "The rationale behind these combinations lies in the different nucleation theories. Since BHN represents the interaction between H_2SO_4 and H_2O , it is a fundamental theory in nucleation mechanisms that exists in most environments (Sipilä et al., 2010). THN represents the involvement of H_2SO_4 , H_2O , and NH_3 in nucleation, used to explain the higher nucleation rates in the atmosphere (Merikanto et al., 2007).

Therefore, the binary and ternary nucleation scenarios are interconnected. But IMN nucleation accounts for the synergistic interactions among BHN, THN, and ions (Yu et al., 2018; Yu et al., 2020). Consequently, this nucleation mechanism cannot be integrated with BHN and THN scenarios. Given that DMA nucleation, containing H₂SO₄ and dimethylamine, has been identified as the predominant nucleation mechanism in urban environments (Yao et al., 2018; Liu et al., 2021; Wang et al., 2021), this study specifically addresses urban nucleation mechanism. Therefore, the DMA nucleation scheme must be incorporated into the combined scenarios. Based on the discussed above, we have retained only two combined scenarios for further analysis."

References:

- Liu, L., Yu, F., Du, L., Yang, Z., Francisco, J. S., and Zhang, X.: Rapid sulfuric acid-dimethylamine nucleation enhanced by nitric acid in polluted regions, Proc. Natl. Acad. Sci. U. S. A., 118, e2108384118, 10.1073/pnas.2108384118, 2021.
- Merikanto, J., Napari, I., Vehkamäki, H., Anttila, T., and Kulmala, M.: New parameterization of sulfuric acid-ammonia-water ternary nucleation rates at tropospheric conditions, J. Geophys. Res., 112, D15207, 10.1029/2006jd007977, 2007.
- Ning, A., Shen, J., Zhao, B., Wang, S., Cai, R., Jiang, J., Yan, C., Fu, X., Zhang, Y., Li, J., Ouyang, D., Sun, Y., Saiz-Lopez, A., Francisco, J. S., and Zhang, X.: Overlooked significance of iodic acid in new particle formation in the continental atmosphere, Proc. Natl. Acad. Sci. U. S. A., 121, e2404595121, 10.1073/pnas.2404595121, 2024.
- Sipilä, M., Berndt, T., Petäjä, T., Brus, D., Vanhanen, J., Stratmann, F., Patokoski, J., Mauldin, R. L., Hyvärinen, A.-P., Lihavainen, H., and Kulmala, M.: The Role of Sulfuric Acid in Atmospheric Nucleation, Science, 327, 1243-1246, doi:10.1126/science.1180315, 2010.
- Wang, Z., Liu, Y., Wang, C., Jiang, S., Feng, Y., Huang, T., and Huang, W.: Multicomponent nucleation of malonic acid involved in the sulfuric acid dimethylamine system and its atmospheric implications, Atmos. Environ., 267, 118558, 10.1016/j.atmosenv.2021.118558, 2021.
- Yao, L., Garmash, O., Bianchi, F., and al., e.: Atmospheric new particle formation from sulfuric acid and amines in a Chinese megacity, Science, 361, 278–281, 10.1126/science.aao4839, 2018.
- Yu, F., Nadykto, A. B., Luo, G., and Herb, J.: H₂SO₄–H₂O binary and H₂SO₄–H₂O–NH₃ ternary homogeneous and ion-mediated nucleation: lookup tables version 1.0 for 3-D modeling application, Geosci. Model. Dev., 13, 2663-2670, 10.5194/gmd-13-2663-2020, 2020.
- Yu, F., Nadykto, A. B., Herb, J., Luo, G., Nazarenko, K. M., and Uvarova, L. A.: H₂SO₄–H₂O–NH₃ ternary ion-mediated nucleation (TIMN): kinetic-based model and comparison with CLOUD measurements, Atmos. Chem. Phys., 18, 17451-17474, 10.5194/acp-18-17451-2018, 2018.
- Zhao, B., Donahue, N. M., Zhang, K., Mao, L., Shrivastava, M., Ma, P., Shen, J., Wang, S., Sun, J., Gordon, H., Tang, S., Fast, J., Wang, M., Gao, Y., Yan, C., Singh, B., Li, Z., Huang, L., Lou, S., Lin, G., Wang, H., Jiang, J., Ding, A., Nie, W. i., Qi, X., Chi, X., and Wang, L.: Global variability in atmospheric new particle formation mechanisms, Nature, 10.1038/s41586-024-07547-1, 2024.