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Comment on acp-2022-797

Anonymous Referee #1

Referee comment on "Analysis of new particle formation events and comparisons to simulations of particle number concentrations based on GEOS-Chem-advanced particle microphysics in Beijing, China" by Kun Wang et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2022-797-RC1>, 2022

This study reanalyzed an NPF dataset reported in previous literature and explored possible nucleation mechanisms by contrasting measurements to simulations. It is interesting to see an attempt to reproduce urban NPF events with a global chemistry transport model. The topic of this study fits the scope of Atmospheric Chemistry and Physics. I recommend the authors take advantage of the review process to improve the manuscript substantially, such that it can meet the quality for publication.

Major comments:

1. The TIMN scheme was found to be able to "overall well simulate the total and sub-3 nm particle number concentrations and nucleation rates in Beijing", with significantly higher values than BHN, BIHN, and THN. However, the nucleation rates in Fig. 10 seem to be lower than typical values in polluted megacities. For instance, the formation rates of freshly nucleated particles were usually higher than $10 \text{ cm}^{-3} \text{ s}^{-1}$ in Shanghai (Yao et al., 2018) and Beijing (Yan et al., 10.1029/2020GL091944). Since the rate of ion-mediated nucleation may be limited by the ion production rate, as well as the high sink, does this indicate that ion-mediated nucleation may not be able to produce those high formation rates? Besides, it will be more convincing to show the measured particle formation rate in Fig. 10.

2. There might be a large room for improvement in the manuscript when addressing the current knowledge of NPF in terms of both nucleation mechanisms and their roles in the atmosphere. Some important advances in the last decade are missing from discussions. There are quite many places where the discussions are confusing and some are even at the risk of self-contradictory. Two examples are given below and some are given in minor comments, and I encourage the authors to improve the manuscript thoroughly.

- Amines can be a key base for sulfuric acid nucleation in polluted megacities for their much higher efficiency in stabilizing clusters than ammonia and ions, as has been discussed in Yao et al. (2018) and many other studies. The authors have cited Yao et al. (2018) but why not address the roles of amines in the simulation? Is it possible that sulfuric acid-amine nucleation can produce a comparable or higher nucleation rate than

TIMN?

- The authors stated that LVOCs play an important role in NPF, which is plausibly true and consistent with previous findings in Beijing. However, it is also stated that "TIMN scheme has a good simulation performance on the growth, condensation, coagulation and other processes after the nucleation process." Have the LVOCs been accounted for in TIMN? If not, does this indicate either a negligible contribution from LVOCs or a bias in the simulation results?

3. Most of the findings in the measurement part have been discussed in previous literature, which can also be seen from the discussions in the main text. The authors may need to clearly show the advances of this study compared to previous studies, including but not limited to the source of the dataset used in this study (Cai et al., 2017). Shortening the discussions, figures, and conclusions based on the measurement results can be an alternative way, and this will help emphasize the results based on simulations.

Minor comments:

4. Lines 55-56. This sentence is confusing because whether ions, specifically, charged particles measured by NAIS herein, grow faster than neutral particles or not is not directly relevant to the formation of the critical nucleus.

5. Lines 60-64. The mechanism proposed by Wu et al. (2020) is not a nucleation mechanism. It will be better to address it elsewhere, e.g., in lines 230-240.

6. Line 213, "7 % higher". It can be questionable to conclude the importance of temperature on NPF based on a 7 % difference.

7. Lines 296-297. Better to explain why and how a nucleation scheme can simulate the processes after nucleation.

Technical comments:

8. Lines 40-41. It is worth double-checking whether Huang et al. (2020) and Li et al. (2021) concluded that "new particles derived from NPF played a significant role in the formation of haze".

9. Line 130. Better to use steady-state or quasi-steady-state. NPF cannot reach an equilibrium.

10. Line 138, "banana shape". This is perhaps not necessary since NPF events in urban environments may not be banana-type events.

11. Line 342. Please use "TIMN scheme" instead of "TIMN nucleation scheme", as N is for nucleation.