Atmospheric Measurement Techniques Discussions

Atmos. Meas. Tech. Discuss., referee comment RC2
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Comment on amt-2022-88

Anonymous Referee #1

Referee comment on "Modelling ultrafine particle growth in a flow tube reactor" by Michael S. Taylor Jr. et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2022-88-RC2, 2022

General Comments

This manuscript describes a modeling study of aerosol growth in a flow tube reactor. The authors frame the discussion in terms of a new quantity they have introduced: the growth yield, which is a measure of the fraction of molecules generated in a flow tube reaction that contribute to particle growth. It can depend on various parameters such as rates of reaction, reactant concentrations, particle size and concentration, particle-phase reactions, etc. Here they show how these different parameters affect the growth yield, and describe how one can use that to extract information from measurements of particle size change in a flow tube reaction.

I find the concept and its value a little difficult to grasp, but as it becomes more widely used I expect that to become more apparent. Some of the difficulty may have arisen because the model was not applied to any measurements in this paper, since that has been done previously. The presentation is well done and the authors provide a clear discussion of the results and interpretation. My primary questions have to do with how many different ways one can accurately model a rather limited set of experimental results. I worry that because of the complexity of most reaction systems that it is difficult to constrain the model. I state some of these concerns below, but there are certainly other issues one would wonder about capturing in a model. I think the approach is novel, and may find use in the aerosol community, and so is appropriate for publication in AMT after the following minor comments are addressed.

Specific Comments

- Why don’t the more volatile SVOCs contribute to the growth yield? Even though they are more volatile, they have higher concentrations and because dimer formation is fast it seems like enough should partition into particles that they can form non-volatile dimers.

- How well are the rates of loss of products to the walls understood, and how does this impact the modeling? Is it irreversible or reversible, and won't this also depend on how much organic or water is on the walls?
- What happens to the model when dimer formation is treated as reversible instead of irreversible?
- Isn't water likely to affect the dimer formation process, for instance completing with hydroperoxides in dimer forming reactions with aldehydes, or shifting equilibria of dimer formation by dehydration reactions?
- It is thought than aerosol particles often exist as phase separated organic/aqueous solutions. Can the model capture this?

Technical Comments

- Line 157: Should be "recursively".
- Line 190, Equation 7: The text in parentheses is not clear.