Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2020-81-RC1, 2020
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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Role of black carbon in the formation of primary organic aerosols: Insights from molecular dynamics simulations" *by* Xiaoqi Zhou et al.

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Received and published: 3 March 2020

This succinct paper used molecular dynamics simulations to investigate the physisorption of gaseous organic molecules on the surface of a carbon nanoparticle. The pollutant molecules were found to cluster in different ways in the presence of the NP than in the gas phase. Authors also suggested a layer-by-layer formation process of aerosol PM, consistent with the onion-like nanostructures of aerosol particles observed before. The topic studied is highly related to the scope of ACP, and results found should be interesting for atmospheric researchers. I suggest the paper is accepted for publication in ACP after some minor issues are addressed.

General comments:

1. Most importantly, it would be nice to see more discussions about the implications of this study for our atmospheric environment. Readers of ACP will like these contents.

2. Figures in the paper are monochrome. I am not sure if it is the problem of submission system. Colored pictures are preferred.

3. Authors used a bucky-onion of 3.64 nm in diameter containing four concentric fullerene layers to represent the carbon nanoparticle in the simulation. The reason of choosing this size was also given: "The system size is kept small due to computational cost considerations, even though BC particles in urban atmospheres can grow from tens to over a hundred nanometers after mixing with other compounds through atmospheric aging processes". As the size of nanoparticles play a key role in the behavior of particles in the sub-10 nm region, I suggest authors to do a series of simulations: one species of organic molecule on the surface of particles with different diameters. Authors can just do simulation and check if the findings based on 3.64 nm particles are still working. If authors do not like to do it, please make it clear why in the paper.

4. In line 80, authors claimed that "A key coefficient influencing the clustering of molecules, the per-molecule binding energy ε is calculated". I suggest authors give more descriptions about this parameter, e.g. explaining why you choose it.

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