EGUsphere, referee comment RC1
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# Comment on egusphere-2022-143

Anonymous Referee #1

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Referee comment on "MultilayerPy (v1.0): a Python-based framework for building, running and optimising kinetic multi-layer models of aerosols and films" by Adam Milsom et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-143-RC1, 2022

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This work developed an open-source framework MultilayerPy to build and run kinetic multi-layer models. Researchers can utilize this framework to choose a certain reaction scheme, diffusion regime, and model component based on particular aims. It is a reproducible process. Local and global optimization are applied and further tested on the oleic acid-ozone heterogeneous reaction system. The work is well-presented, and the framework makes comparing aerosol models with experiment data easier. I have one major comment and several minor comments.

Major comments:

Overall, the quantity of case studies is insufficient to assess the framework's potential applications. For example, current case studies are not convincing in testing the multi-layer modeling ability of MultilayerPy. As shown in figure 3, there is no oleic acid concentration gradient between the layers. Could the authors provide more cases to test the ability to represent the layer differences? Also, will it be easy to find other reaction systems to test the differences between KG-SUB and KM-GAP? and how the optimization algorithms will address the differences?

Minor comments:

Line 29--33: Consider including more references about the specific scientific questions KM-SUB and KM-GAP have resolved. That can be the potential application of MultilayerPy.

Line 54: typo ``readable''

Line 62: I think the flexibility of adding unique processes to the framework is an important feature. However, the steps to achieve this are not well-documented in the rest of the paper. I recommend adding some descriptions about this at the steps listed in lines 93--100.

Figure 3: Would it be better to combine (b) and (c) together? It will make the differences more evident.

Line 252: Besides the codes, it would be easy for readers to follow if the steps to create the cases are briefly documented.

Line 280: How did you get the optimized value of $\alpha_{\rm s,0, ozone}$? Did you use the same model data used for the MCMC sampling procedure? I am thinking of training and validating data differences in Machine learning.