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Comment

***Interactive comment on* “Estimation of aerosol  
particle distributions with Kalman Filtering – Part  
1: Theory, general aspects and statistical validity”  
by T. Viskari et al.**

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Dear anonymous referee #2,

Thank you for your review of our article and your reasonable commentary.

First to response to your primary concerns, we did not use a time-filtered inverse solution, because we wanted to compare the results to the currently used inversion method for Hyytiälä measurements. As our research has been about the application of EKF in combining observations, we did not further develop the current inversion methods as that was not a part of our research.

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As for the validation of the method with independent observations, we did not consider that feasible. The true state is not known and all other measurements will also contain uncertainties. Thus the state estimate  $x_{EKF}$  was compared directly to the DMPS raw observations  $y$ . The residual  $r=y-Hx_{EKF}$  has to meet two conditions: i) the bias and standard deviation of  $r$  has to be in the equal or better than the residual computed from the mathematical inversion, ii) large values of  $r$  are either due to measurement noise or special circumstances (e.g., precipitation, change of air mass). Because the true state is not known, this validation is admittedly subjective, but we feel that the set standards were reasonable as to establish the validity of the estimate.

Then for the specific comments:

“Title: The title of this paper is different from the authors’ Part 2 paper. The term “aerosol particle distributions” is vague. “aerosol particle number distributions” or “aerosol particle size number size distributions” should be used.”

You are correct and we changed the term to “aerosol particle number distributions”.

“P 18855, line 26: Liu et al. is the error of Lin et al.?”

It was an error, thank you for pointing that one out. We changed it to Lin et al.

“P 18857, eqs (1) and (2): Why do you include the error term  $Q$  in eq (2) but not include an error term in eq (1)? Standardization is recommended. Plus,  $Q$  represents not only system noise but also the model “imperfection” error.”

Equation 2 represents the uncertainty of the state calculated in equation 1, essentially being the error term of equation 1. Additionally, as equation 1 represents the expected value of background state, it should not include the error term. As for  $Q$ , you are correct that it does not just contain the system noise. We have added to the article that it also contains errors due to model discrepancies.

“P 18859, line 24: What is “transfer function peak diameter?”

MA transfer function defines the probability of particles of certain electrical mobility to pass through the DMA instrument. It has a triangular shape with the peak corresponding to the best represented mobility. This mobility can be converted to size assuming the particles are singly charged. This "peak diameter" is then the most likely particle diameter entering from the DMA with the selected voltage.

"P 18860, section 3.2: Please describe the model initialization in this section, not in section 4.2."

The system initialization described in section 5 (We assume you are referring to that) covers more than the model initialization requested here. We, however, added to this section how the model is initialized as well as how it is re-initialized after each observation update.

"Is R in Eq (7) supposed to be the same as R in Eq (6)?"

Yes. We added a sentence to clarify this.

"P 18861, line 22: Please describe the more detailed validation process of "a mathematical inversion" method, or draw references."

We did not include the validation process here, as here we simply stated how we tested the observation operator by showing that it produced values close to the observations from a solution obtained in a different manner. We did, however, add a reference to Wiedensohler et al. (2012) to section 3.1 and mentioned how the mathematical inversion solution is validated there.

"P 18864, line 9-12: This sentence is very vague. Don't you mean that the smallest particles and the largest particles are correlated?"

No, at least not exactly. What we meant was that there is a notable correlation between particle sizes smaller than 10 nm, where most of the particles are newly formed particles, and particle sizes which have the largest combined surface area, thus affecting the ambient vapour concentration most. We tried to clarify this in the sentence.

“P 18864, line 20: “a large innovation can only affect the size distribution to a maximum distance of 15 size bins.” This method is called “variable localization”, which is sometimes used for ensemble Kalman filters.”

Thank you for mentioning that. We added this to the article as well as a reference to Hamill et al. (2001).

“P 18865, line 15: The phrase “in Fig. 2” appears twice in this sentence”

Thank you for pointing that out. Corrected.

“P 18865, line 18: Xekf is smoothed, and Xinv is apparently noisy. But it is not clear that Xekf is less erratic than Xinv.”

You raise a valid point here. By mentioning the Xekf being less erratic than Xinv, we meant the edges of the distribution, where the Xinv shows much more random changes than Xekf. However, there are large changes in the size distribution over the day which are not always continuous and thus seem erratic at times. We decided to remove the reference to Xekf being less erratic as we agree that it might seem confusing.

P 18865, line 21: “which makes it difficult to limit Xekf to the same diameter range than Xinv” I do not understand what this sentence means: : : You are correct in the sentence being unclear. We meant that in order to compare the total number concentration of Xekf and Xinv, the total number concentration must be calculated over the same particle diameter range. However, as the size bin diameters for Xekf and Xinv are not the same, it is difficult to set the lower limit for Xekf as the same than the lowest diameter of Xinv. This partially causes the larger total number concentration for Xekf. We changed the text to better explain this.

“P 18866, line 5: The observations could have biases. Otherwise, the observation overlap must improve the data assimilation result even if the observations have random noises.”

This is what we essentially meant in the text. It is evident that the disagreement be-

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tween the two DMPS:s is not random, as they have distinctive biases.

“P 18866, line 7 and Fig 3: The x-axis is expressed by the unit of m, but the text is described by the unit of nm. This discrepancy is not reader-friendly. Standardization is recommended.”

We used the unit of m in Fig. 2 as it we felt it suited the logarithmic scale better. Thus we also chose to use, for the sake of standardization, the unit of m in all the figures. In the text, however, we felt that it is easier to refer to nanometers than 10-9 meters. We would thus keep the current expression of units, as we feel that is largely understandable and easier to understand.

“P 18866, line 13: The phrase “broadly equally large” is vague. What is equally?”

We meant that the standard deviation are approximately as large for Xekf and Xinv. We changed the text to say this.

“P 18866, line 13: I have no idea that the standard deviation is large or not, because the values of raw measurements are not shown in this section.”

We are not saying that the standard deviations are large compared to the raw measurements, but that when compared to each other they are of the same size.

“P 18867, line 11: If you think that large random errors in observations are excluded in the EKF result but included in the inversion result, why did not you use a time-filter to smooth the observations or the inversion result?”

The inversion results were not time-filtered, because the currently used inversion method does not time-filter them. Besides, the time-filter would also require assumptions and testing while having included uncertainties. As for the observations, as the EKF already reduces the impact of large random errors in the observations, we felt that we did not want to additionally alter the observations themselves.

“P 18867-18868, section 5.2.1: Generally, Kalman filters are not good with sudden

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changes in the system state. However, Kalman smoothers are good at following such sudden state changes because they can use the future observations. If you are not going to use this EKF system in real time in the field, using extended Kalman smoothers is a good choice.”

We hope to create an implementation that could be used in real in the field, thus the choice of the Kalman filter. Additionally, while Kalman smoothers do have their advantages, especially in the case of sudden changes in state, they also have their drawbacks. For example in the case of the sudden change in system, the smoother would have state estimates prior to the change already include information from the new system.

“P 18869, line 4: If a noise filter was used for the raw measurements or the inversion results, you could prove your story.”

We based our argument on the random noise being the prime source for the large standard deviation for xEKF by studying subsequent observations and determining what was causing the difference between the estimate and the observations. If we had used time-filtering, we would have had to do something similar to ascertain that the differences were due to measurement noise. Thus our argument was not based on simple assumptions.

“Captions of Figs 2a and 3a: “1” before the unit is unnecessary in the International System of Units (SI). For example; “1m-3” -> “m-3”; “[1 cm-3]” -> “[cm-3]””

True. Thank you for pointing that out and it has been corrected in the article.

References:

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