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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Estimation of aerosol particle number distribution with Kalman filtering – Part 2: Simultaneous use of DMPS, APS and nephelometer measurements" *by* T. Viskari et al.

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Dear anonymous referee,

We begin by thanking of your thoughtful commentary on our articles. Your arguments are justified and well-presented. It appears that the main disagreement here is over the appropriateness of UHMA as the forward operator, which we address further below. We also understand the issues with the super-micron measurements and did discuss the matter before writing the articles. We explain our reasoning concerning the different points raised in the review in the same order as they were raised.

1. The air mass changes: The reviewer is correct that UHMA is a 0-dimensional box

model and is as such designed for a Lagrangian system while the measurements are done in an Eulerian environment. We also admitted in the discussion section of the first part of the articles that both discontinuities of the measurements and flaws in the microphysical model are current challenges in the implementation of the EKF. This was one of the reasons we chose measurements for 7 May 2007 for the initial testing as it contains multiple sudden changes in the aerosol size distribution. We also tested the EKF implementation with measurements from several days with different particle number size distribution evolutions.

As discussed in Part I, while major changes in the particle number size distribution did occur in the measurement periods, they were still relatively rare and EKF was able to adjust to those large changes in the system over approximately 2-3 subsequent measurements. We considered this to be a relatively fast adaptation to the new state in the system. Besides those large changes in the system, the EKF implementation was able produce continuous state estimates for concurrent measurement times that fit the available observations, with the natural exception of apparent measurement noise. Thus we argued, and still argue, that EKF was a valid method to estimate aerosol particle number size distributions from in-situ measurements. Additionally, it is important to note that the sudden changes in the particle number size distributions also cause difficulties for smoothing methods, which are nevertheless already applied with aerosol measurement series.

Furthermore, we disagree that the EKF implementation cannot have the capacity to react to the sudden changes. There are at least two methods we are considering to improve the state estimate adaptation to air mass changes. The first option is to use the ambient measurements (temperature, pressure, wind, etc.) to detect changes in the air mass, as those ambient conditions should also change when the air mass changes. The second option requires us to improve our understanding of associated uncertainties. In essence we could determine when the differences between the background state and observed state are statistically significant enough for the EKF implementation to recognize as them as different size distributions. In both cases, the EKF implementation could then basically re-initialize the application and thus quickly adapt to change. We expanded in to the discussion part of the first part explanation on how, in the future, we can improve the EKF implementation's adjustment to the sudden changes in the system.

2. & 3. We will address all your points concerning the super-micron range here together. Your concerns about the estimate in that size range are valid, although there was a slight misunderstanding concerning one of our assumptions. We do not place any minimum limitations to a number concentration in a size bin. What we discussed in the article was that in order for us to avoid instabilities when calculating the inverse matrix required by the Kalman Filter, we added a small fixed value to the diagonal. The impact of this addition was largely mitigated by ignoring the smallest eigenvalues when applying SVD to determine the inverse matrix. Secondly, you are correct that the limit of 90 % decrease of the background state is an artificial, ad hoc solution. However, in our tests, we did not come across situations where this greatly prolonged the effects of a natural large spike in measurements. Additionally, as the value is the limit is artificial and simply inserted to prevent the state estimate from containing negative number concentration values, the limit can be increased to a large value as long as it smaller than 100 %. Thus it can easily made large enough to account for sudden spikes in measurements.

However, that said, your point about the error in those particle sizes not being Gaussian is completely valid. This is a problem we realized during testing and discussed to some length, as it has no doubt an effect on very low concentration measurements. For example, for this reason we excluded information from zero measurements from affecting the state estimate as the Gaussian uncertainty is clearly false there. Limiting the included measurements, though, based on if the error for them can be considered Gaussian requires improved understanding of the associated uncertainties both the background state and the observations. Thus we did not discuss the matter here.

You are also correct on the estimation problems for larger particles. The wind effect in the larger particle sizes is a major problem for the method, although we had not previously considered the gravitational settling as an additional potential problem in very large particle sizes. We attempted to discuss the problems with the state estimate for particles larger than 5 micrometers, but did not focus there as it is not the main size range of interest in the article, especially with the acknowledged problems with the measurements and model in that size range. However, we were, and still remain, optimistic that EKF could provide a reasonable estimate even in those particle sizes even though the associated uncertainties would still remain large. This would, though, requires us to first address the number concentration limit for which the associated uncertainty can be considered Gaussian.

We have made the following changes to the article. We added in the discussion section of the first part a point about the possibility of the non-Gaussian error. In the second part, we mentioned the Poissonian error problem when discussing the problems with estimate for particle sizes larger than 4 micrometers. We did not specifically stress how better observations and error approximations are needed to improve the estimate in these particle sizes, as that does hold true for the whole state estimate.

Lastly we feel the need to explain that even though the changes in the articles are small, we did not ignore your concerns and points. The key disagreements, however, seem to be on a more fundamental level, such as can UHMA be effectively used in these conditions. As we feel that it can be used in these conditions and that our results support this assumption, we have instead tried to explain our justifications in this response.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 18889, 2012.