Response to A.M. Sayer

I have a few questions/comments about the approach taken in this paper. In general I think that a simultaneous atmosphere/ocean inversion like this is a good way to go, and Optimal Estimation is a good inversion technique to apply for a problem like this. The application to data within Sun glint is also interesting. But I had some questions about the details which I didn't spot in the manuscript (perhaps I missed something).

Dear Sayer, we appreciate your comments very much, which helped improve our manuscript greatly. We have revised our paper based on your comments carefully. We also have reworded/rephrased some sentences and added some references that may improve the paper. Our responses are listed in below after each comment.

A strength of Optimal Estimation is the uncertainty estimates provided (Equation 7), as well as the ability to use a priori data. The authors note the a priori values for parameter, but I don't see the a priori uncertainties anywhere (except for Chl where it is noted to be the variance of the standard MODIS product). What are they? Likewise, I am curious what the averaging kernels look like for these retrievals. Al-though one can retrieve 8 things from 8 measurements, considering that there is a high degree in spectral correlation between the measurements, there must be far fewer than 8 degrees of freedom. So it is likely to me that there are degenerate solutions, large null space uncertainties (hinted at for e.g. wind speed outside of glint, in Figure 7), and/or strong dependence on the a priori assumptions in some cases. For example I wonder if some of the skill for the aerosol composition is coming from a tight constraint to the SPRINTARS model?

Response: Thanks for the comments. We agreed that the degrees of freedom are fewer than 8, actually about 3.5~4.5 in this study. In general, a higher averaging kernel values are existed for the retrieval of AOT, sediment and CDOM than that of soot fraction, wind speed and Chl. Therefore, we use the NCEP wind speed, annual average MODIS Chl in 2009, SPRINTARS AOT and soot fraction as the apriori constraint. For the AOT of fine particle, sea salt and dust, as well as soot fraction in fine particle, the monthly averaged aerosol products of SPRINTARS global simulation from 2007 to 2009 are used as apriori and uncertainties values. The uncertainties values for wind speed, sediment and CDOM are 0.5 m s^{-1}, 1.0 g m^{-3} and 0.1 m^{-1}, respectively. Indeed, the retrieved wind speed value is strongly dependent on the apriori values when the measurements are out of sun glint, but it has little effect on the satellite reflectance in such cases except sun glint contamination. In addition, the soot fraction in fine particle is still difficult to be determined due to the weak sensitivity to observation (maybe without adequate ultraviolet bands information) and also dependent on the apriori values in most cases. Moreover, since we focus on the retrieval of spectral nL_w instead of concentration of oceanic components, the Chl, sediment and CDOM are just three parameters to adjust the spectral L_w, of which detail values are less important.

It would also be useful to include the uncertainty estimates on retrieved parameters on the validation results shown in e.g. Figure 4. That way we can see whether they are reasonable or not. Figure 7 shows simulations but since there is validation shown with real data, it would be good to see the uncertainty estimates for these real data as well.

Response: Thanks a lot. It is a good idea to include the statistical uncertainties on retrieved parameters for the validation results. Eq. (7) can be used to determine the estimated uncertainty for parameters that are retrieved, as well as parameters that are not directly retrieved if they can be expressed by the state vector $\mathbf{x}$. Since we directly retrieve the AOT for each particle and concentrations of oceanic substances, an equation is used to determine the estimated uncertainty for total AOT and spectral nL_w as follows,

$$\sigma_a = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n}\hat{\mathbf{S}}_{i,j}\frac{\partial a}{\partial x_i}\frac{\partial a}{\partial x_j}}$$

where a is a parameter that are not directly retrieved, i.e. total AOT and spectral nL_w in this study.

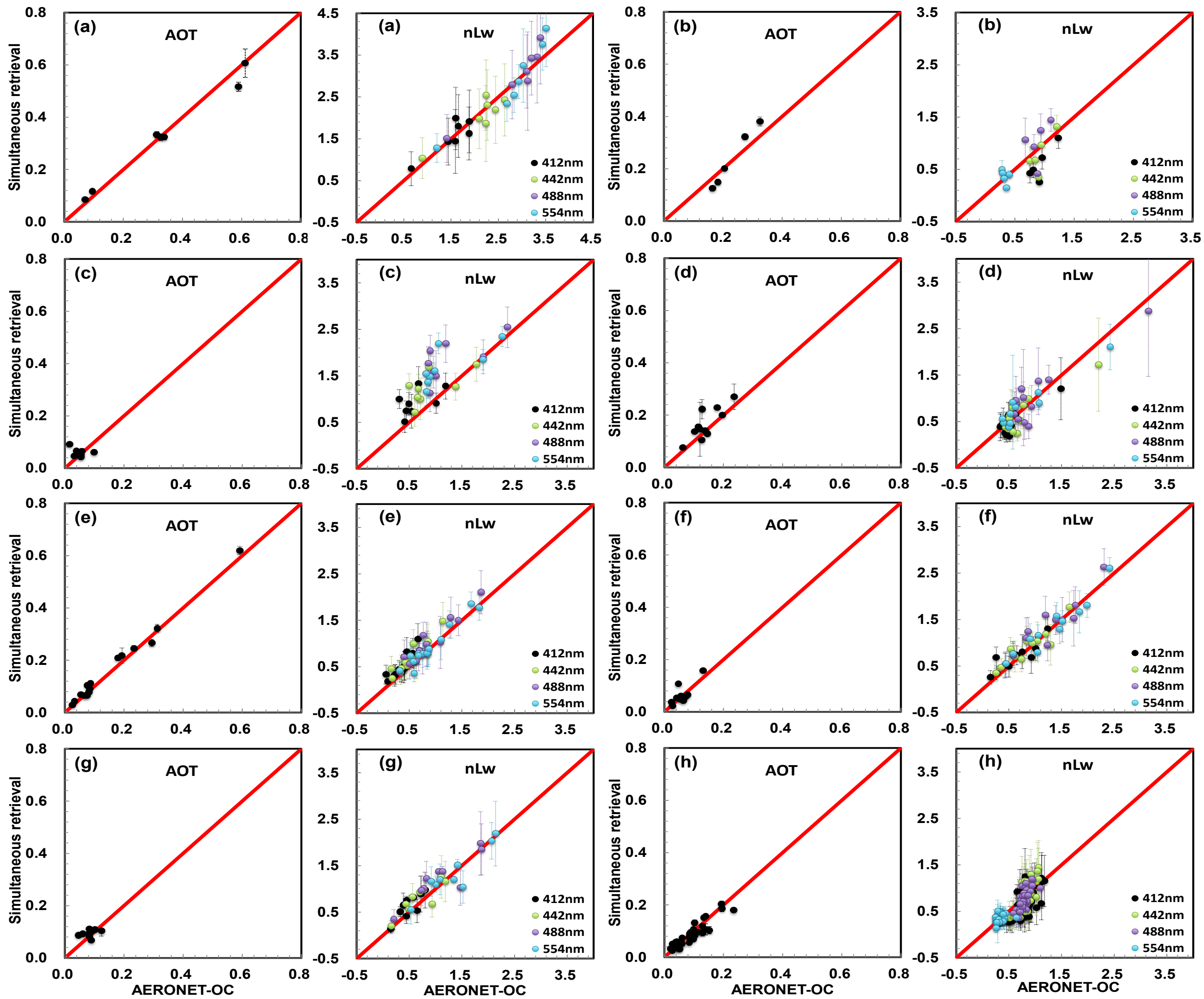

Figure: Comparison of satellite simultaneously retrieved AOT at 550 nm and nLw (mw sr-1 cm-2 μm-1) with AERONET-OC observations. Red line represents the 1:1 line (a: Ieodo_Station; b: GOT_Seaprism; c: Lucinda; d: Abu_Al_Bukhoosh; e: Galata_Platform; f: COVE_SEAPRISM; g: Thornton_C-power; h: USC_SEAPRISM).

I suggest adding the MODIS 1.2 and 2.1 micron bands as well. These will not have much ocean colour information, but may help better constrain the aerosol contribution to the signal. By increasing the number of measurements relative to retrieved quantities, this should in general decrease any degeneracies in the retrieved state.

Response: Thanks. We only use one shortwave infrared (SWIR) band in this study just want to estimate the ability and flexibility of algorithm in turbid waters, so that it can be used to other satellite instruments with only one SWIR band, such as GOSAT2/CAI2. We also do the retrieval adding 1.2 and 2.1μm bands, the retrieved nL_w are improved generally, particularly for nL_w at 488 nm, however, the accuracy of retrieval AOT at relative clear waters, such as at USC_SEAPRISM sites, are decreased, which inspiring us to optimizing the aerosol or oceanic module again.

I am curious how the minimisation actually works computationally (I did not see this mentioned in the paper). Is it a minimisation from a multidimensional lookup table? Or is the radiative transfer code called for each iteration of the retrieval? If it is a lookup table, is the full atmosphere/ocean state included in the simulation (which is the most accurate but then requires a higher-dimensional lookup table) or is there some assumption like linear mixing to include the contribution from multiple aerosol components more simply? Linear mixing is used in e.g. the standard MODIS AOT product for computational efficiency, but has systematic biases when there is absorption in the atmosphere. See Abdou et al (1997, http://onlinelibrary.wiley.com/doi/10.1029/96JD03434/abstract) for some discussions of limitations of linear mixing and a modified method (which decreases, but does not eliminate, this error source).

Response: Thanks for the comments and reference introduction. The coupled atmosphere-ocean radiative transfer code is called for each iteration in this study. We agree that the lookup table will require a higher dimensionality with huge size volume for this study, particularly that a lot of parameters are needed to be retrieved and determined in advanced (actually about 15 parameters in this study), thus, a Neutral Network Solver (Takenaka et al., 2011) is being trained to replace the RT model as a result that the calculation efficiency is expected to be increased over thousand times and no LUTs are needed. Such work will be elaborated in another paper.

What is the first guess at the retrieval solution? Is this initialised from the a priori value?

Response: We define low values of state vector (0.01) for the first guess of retrieved parameters except wind speed from a priori value.

Page 7, lines 15-16: I do not understand this sentence. Is the soot fraction in fine particles retrieved (as stated in line 15) or assumed (as stated in line 16)?

Response: The soot fraction in fine particles is also retrieved in this algorithm. As the previous explanation, it is still difficult to be determined currently.

For the vicarious calibration, are 18 points really enough to state with confidence that there is no significant temporal or geometric dependence in the results? What are the uncertainties on the derived calibration coefficients? Also, are the Werdell (2006) results shown in Figure 3 the latest coefficients used in the MODIS ocean colour algorithm? There have been numerous reprocessing since then and calibration coefficients have changed. I looked at the MODIS webpage and the calibration gains there for the 2014 Aqua reprocessing (https://oceancolor.gsfc.nasa.gov/reprocessing/r2014/aqua/), which I think is the latest, are different. I think it is also worth stating up front as well that the vicarious calibration effectively calibrates out the average bias in the sensor plus forward model at the calibration site, as some readers may not be aware of this. This in turn means that biases can be introduced in conditions which are different from those at the site used to tune the data in this way.

Response: Thank. It is studied that the derived gain factors show no significant temporal or geometric dependencies, and the mean values can be stabilized after approximate 20 high-quality calibration samples (Franz et al., 2007). In this study, we make a strict data screening criteria followed by Franz et al. (2007), and adopt the observed AOT at 550 nm and spectral nL_w products of AAOT site for vicarious calibration, which is similar to the study of Yoshida et al. (IEEE transactions on geoscience and remote sensing, 2005). We add 12 data with number of 30 points for the vicarious calibration in the revision, and find that the variation of calculated averaged calibration coefficients are generally less than 1% compared with original ones. Since we also use the ground observed AOT at 550nm data for the vicarious calibration, which is different from the standard calibration scheme that only use nL_w observation, such a comparison with the standard calibration gain factors seems to be meaningless and is deleted in the revised manuscript as shown in the below figure. However, it is still a difficult thing to systematically investigate the biases introduced by the used vicarious coefficients derived from other locations currently.

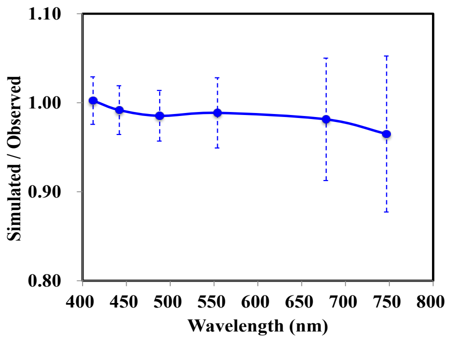

Figure: Averaged vicarious calibration coefficient for each channel.

Figures 5, 8: I would remove the regression lines from these plots. Linear least squares regression is not valid for AOT data because the expected error is AOT-dependent (and type-dependent), the uncertainties are not Gaussian, the points are not independent, sampling is highly skewed to the low-AOT end, and the expected relationship between truth and retrieval is not necessarily linear. So the slope and intercept, and their uncertainties, estimated using this technique are misleading. It is a popular technique but it is mathematically inappropriate for these data.

Response: Thanks. The regression lines of figure 5 and 8 are removed in the revised manuscript.

Although not directly relevant to the point of coupled ocean/atmosphere inversion, since the authors also look at the MODIS ocean colour product, it would be interesting to see the comparison of AOT for the MODIS aerosol products as well. This sort of simultaneous inversion should result in better results than the MODIS aerosol product, since the standard aerosol product does not account for variations in ocean colour (as the authors rightly point out in the introduction). Similarly it should help by having more aerosol information than the standard ocean colour approach, which may alleviate some biases in standard ocean colour prod- ucts. On that point the authors may be interested in the study Kahn et al (2016, http://journals.ametsoc.org/doi/abs/10.1175/JTECH-D-15-0121.1), which assesses some of these contextual biases in ocean colour data.

Response: Thanks for the comments and reference introduction, which is added in the revised manuscript. The below figure shows the comparison of jointly retrieved AOT at 550 nm from simultaneous retrieval algorithm, MODIS OC products and MODIS atmosphere products using satellite measurements out of sun glint with AERONET-OC in situ products. There are only two coincided data from MODIS atmosphere products in sun glint cases and such comparison is ignored. Generally, MODIS atmosphere aerosol products have a best estimation of AOT over 550 nm bands, on the contrary, current algorithm exerts a more accurate retrieval of AOT below 550 nm bands. Since this manuscript focuses on the retrieval of AOT and spectral nL_w, we only show the comparison results from MODIS OC scheme with a clear text structure.

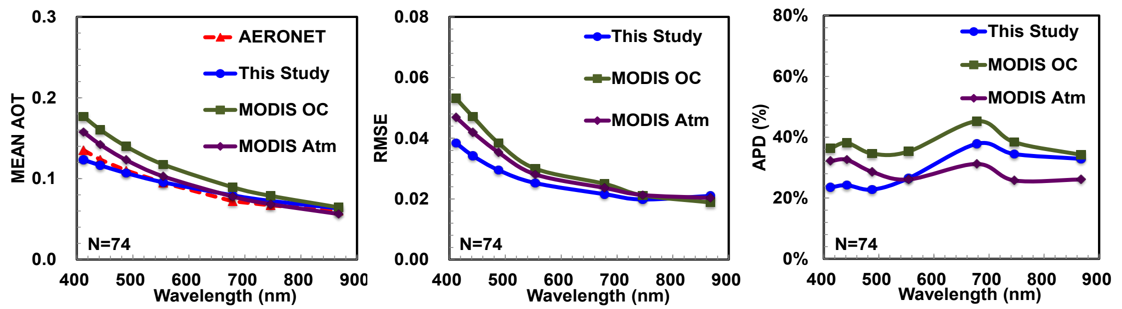

Figure: Statistical mean AOT values, RMSE, and APD results retrieved by these three approaches compared with AERONET-OC products

Finally, it would be interesting to see some mapped results of the algorithm as opposed to just scatter and line plots. I suggest the authors add some case studies with different aerosol/ocean features, and show true colour images together with their retrieved data fields and uncertainties. It would also be instructive to show some of the standard NASA MODIS ocean colour and/or aerosol products, to see whether spatial patterns are consistent, and whether any differences or discontinuities can be related to sur- face/aerosol features not accounted for by one of the algorithms. In particular, since this paper was submitted to ACP and not AMT, it would be good to see more comparison/application of the results rather than just algorithm description and validation.

Response: Thanks for the comments. We add a mapped result for the retrieval of AOT at 550 nm and nL_w at 412 and 554 nm in Fig.8. The following description is added at the end of section 4.2.

"The algorithm is then applied to the selected image obtained around the East China Sea on October 2011. Spatial distributions of the simultaneous retrieval of total AOT at 550 nm, nL_w at 412 nm and 554 nm are shown in Fig. 8(c), 8(e) and 8(g), the MODIS standard aerosol products (Fig. 8(a)) and OC products (Fig. 8(b), 8(d) and 8(f)) are also added as comparisons. In general, the retrieved AOT are mostly similar to that of MODIS aerosol products, as well as OC products, where the high aerosol loading around Bohai Sea can be observed in Fig. 8(a) and 8(c), however, the MODIS AC scheme can not produce useful AOT data in this heavy aerosol area (Fig. 8(b)). In regards to the estimated nL_w at 412 nm and 554 nm, there are also good consistencies between MODIS OC products and those derived from the simultaneous retrieval approach, while the retrieved nL_w at 412 nm from MODIS OC products are reported to be negative values in the north of Yellow Sea (Fig. 8(d)), where such case can be avoided using current scheme shown in Fig. 8(e)."

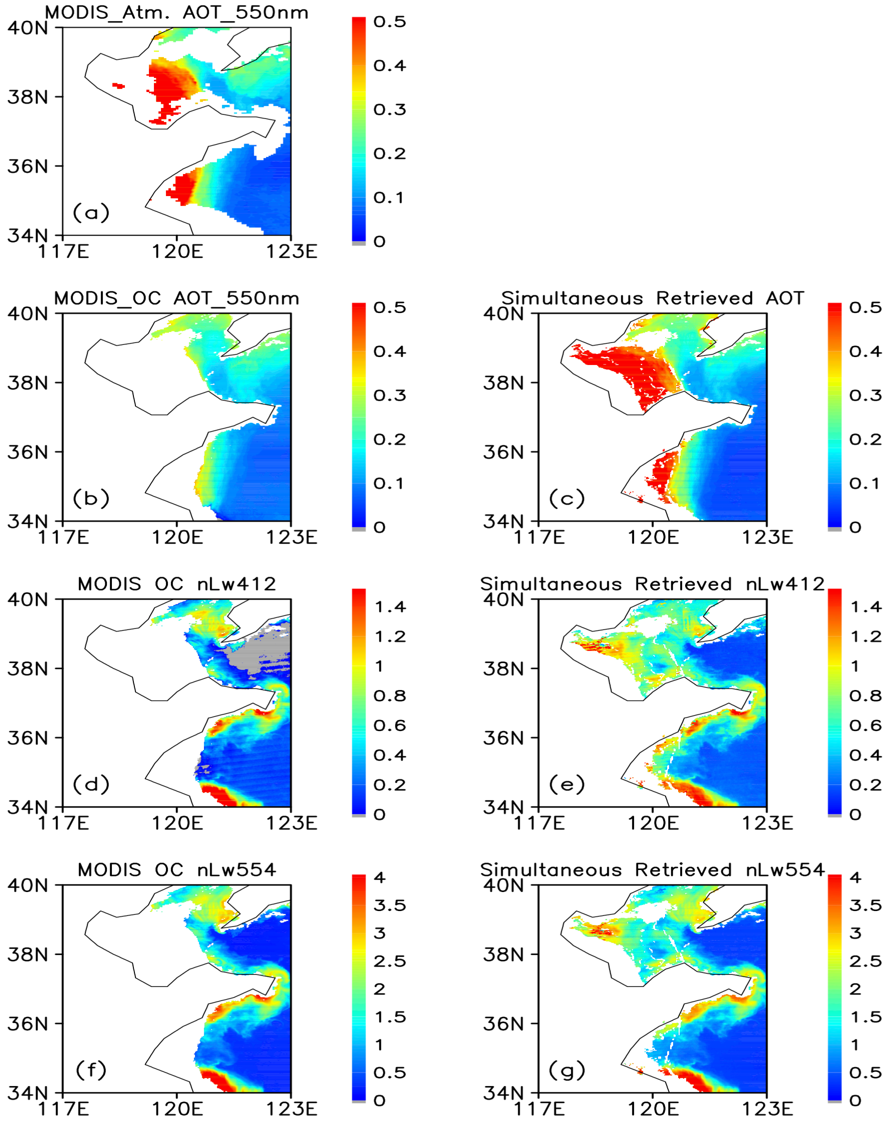

Figure 8: Comparison of satellite simultaneously retrieved AOT at 550 nm and nL_w (mw sr^{-1} cm^{-2} μm^{-1}) at 412 nm and 554 nm with MODSI operational products over East China Sea on 18th Oct. 2011. (a) MODIS Aerosol AOT products; (b), (d), (f) MODIS Ocean Color AOT and nL_w products; (c), (e), (g): Simultaneously retrieved AOT and nL_w in this study.