RC3: 'Comment on amt-2022-112', Anonymous Referee #3

Review of manuscript submitted to AMT:
Title: Effective uncertainty quantification for multi-angle polarimetric aerosol remote sens-ing over ocean, Part 1: performance evaluation and speed improvement
Authors: Meng Gao et al.

General Comments
In this paper, the authors analyze theoretical uncertainty estimates and validate them using a Monte Carlo approach to generate error statistics. A previously developed Fast Multi-Angle Polarimetric (MAP) Ocean coLor (FastMAPOL) retrieval algorithm is used to carry out the retrievals and quantify uncertainties for both synthetic HARP2 (Hyper-Angular Rainbow Polarimeter 2) and AirHARP (airborne version of HARP2) datasets. The FastMAPOL retrieval algorithm is based on neural network (NN) forward vector radiative transfer model (VRTM) simulations pertinent for a coupled atmosphere-ocean system. The NN forward radiative transfer models are trained using synthetic data generated by the VRTM. For practical application of the appraoch to uncertainty evaluation in operational data processing, the authors apply a previously developed automatic differentiation method to calculate derivatives (Jacobians) analytically based on the neural network models. Both the speed and accuracy associated with the quantification of uncertainties for retrievals based on MAP data are presented and discussed. Pixel-by-pixel retrieval uncertainties are evaluated for synthetic data as well as data obtained in AirHARP field campaigns. The authors argue that the methods and results presented in this paper can be used to evaluate the quality of data products, and guide algorithm development based on MAP measurements for current and future satellite systems.

We appreciate your time and efforts in reviewing this work. The comments and questions are valuable in improving the clarity of this manuscript. The responses are below (in red) with manuscript revised accordingly (also uploaded).

The paper is generally well written and the results appear to be robust and valuable. Therefore, I recommend that the paper be published after minor revisions outlined below.

Thank the reviewer for the positive comments.

Specific Comments
• On line 6, the authors mention “nonlinearity of radiative transfer near the solution”.
Since the VRTE is a linear equation, the authors should clarify what they mean here and use proper wording.

Thank you for the suggestion. Here the nonlinearity is referring to the non-linear relationships between the total reflectance and polarization with respect to the retrieval parameters. We revised the sentence as follows:

> “However, standard error propagation techniques in high-dimensional retrievals may not always represent true retrieval errors well due to issues such as local minima and **the**

nonlinear dependence of the total reflectance and degree of linear polarization (DoLP) on the retrieved parameters near the solution."

• line 53: the statement "the forward model is linear near the solution" also needs rewording, because the RTE is a linear equation.

Here we are discussing the assumptions in error propagation. Similar to above discussions, we revised the sentence as follows:

> "…a) the input uncertainty model is sufficient, b) the retrievals converge to their global minimum, c) **the forward model is linear with respect to the retrieval parameters near the solution.**
> "

• line 54: change "With MAPs, theoretical uncertainties...." to something like "For MAP measurements, theoretical uncertainties...."
Thanks for the suggestions. We have revised the sentence as:

> "**For MAP measurements,** theoretical uncertainties have been widely used for aerosol and cloud retrieval algorithms for sensors…"

• Line 62: change "error propagation does but require" to error propagation but requires"
We have revised the sentence as:

> "The 'real' uncertainty does not require the same assumptions as error propagation but **requires** the existence of 'truth' data of high and known confidence,…"

• line 64: change "With MAPs, theoretical uncertainties...." to something like "For MAP measurements, theoretical uncertainties...."
We have revised the sentence as:

> "**For MAP measurements,** real uncertainties have been discussed for aerosols over ocean, land, and cloud by comparing retrievals with synthetic data and in-situ measurements…"

• Line 74: change "Several approaches has been proposed" to "Several approaches have been proposed"
Updated.

• Line 78: explain what "non-linearity around the truth" is supposed to mean
We have discussed the non-linearity in the response to the first two comments.

• change "properties retrieved directly by the MAP" to "properties retrieved directly from the MAP data"

Updated

• "more advanced instruments" please be more specific
We have revised the sentence as below:

"…and can guide further uncertainty studies and algorithm development when more advanced instruments **with higher angular and spectral resolutions** are available."

• Line 114 "Section 4. quantified" → 'Section 4 quantifies"
Updated

• Line 115 "Section 5. quantified" → 'Section 5 quantifies"
Updated

• Line 125: "There are two MAPs on PACE" → "There are two MAP instruments on PACE"
Updated

• Line 147: "lower-dimensionality retrievals" – please explain.
We have revised the term as:
"… as is common for **retrievals with a small number of parameters**,…"

• Line 158: "assumed as a combination of five lognormally-distributed aerosol sub-modes" – please justify this choice

From our previous test with respect to the RSP data, we found the retrieval of the number density of each sub-mode is more robust than directly retrieve the effective size and variance of the aerosol volume distribution. For a more general study, Fu and Hasekamp discussed the representation of aerosol size distribution through various numbers of sub-modes and also found that a similar five-mode approach can provide good retrievals for most aerosol parameters (Fu and Hasekamp, 2018). We have added a sentence to reflect this:

> "The aerosol size distribution is assumed as a combination of five lognormally-distributed aerosol sub-modes, each with prescribed mean radii and variances; the five volume densities (Vi) are free parameters (Dubovik et al., 2006; Xu et al., 2016). **The five-mode approach is found to provide good retrievals for most aerosol parameters** (Fu and Hasekamp, 2018)**.**

• Line 175: "the spectral ocean color remote sensing reflectance (Rrs(λ)) is derived based on the retrieved aerosol properties through atmospheric correction" – a physically more satisfactory and accurate approach is presented by Fan et al. (2021).
Thank you for the reference. We have added it in the manuscript. We also provide more information on why we prefer the atmospheric correction approach. It will be useful to apply the MAP retrieved aerosol parameters to conduct atmospheric correction on other sensors, such as PACE OCI

> "In addition, the spectral ocean color remote sensing reflectance (Rrs) is derived based on the retrieved aerosol properties through atmospheric correction, a procedure to derive ocean color signals by removing the contributions with atmosphere and ocean surface from the top of atmosphere (TOA) measurements (Mobley et al., 2016, 2022). **The atmospheric correction and other associated procedures have been implemented using NNs by Gao et al. (2021) with more details provided in Appendix A. The atmospheric correction method also provides a convenient way to derive ocean color signals from other sensors, such as PACE OCI, using the MAP retrieved aerosol properties. Note that NN method has also been used to directly link Rayleigh-corrected TOA radiances with normalized remote sensing reflectance by Fan et al (2021).**"

• Line 192: "STIR is based on the Levenberg-Marquardt algorithm combined with ..... " – Please summarize the advantage of the STIR method compared to a "standard" Levenberg-Marquardt algorithm.
We have added more discussion as follows:

> "The subspace trust-region interior reflective (STIR) algorithm is employed to conduct non-linear least-square minimization of the cost function (Branch et al., 1999). **Its implementation in the Python package SciPy is used in this study (Virtanen et al., 2020).** STIR is based on the Levenberg-Marquardt algorithm combined with an interior method and reflective boundary technique (Branch et al., 1999). **The interior method ensure that the retrieval parameters are searched strictly within the interior of the feasible region as specified in Table 1, while the reflection technique can significantly reduce the number of iterations in the minimization process.**"

• Equation (14) – a physically more satisfactory and accurate approach consistent with the coupled atmosphere-ocean system is provided by Fan et al. (2021).
We have added the reference and discussed the reason why we are conducting such atmospheric correction in the response to one of the previous comments. Please also note that the section containing the equation has been moved to Appendix A.

• Line 354: "Note that the synthetic data is computed directly using the vector radiative transfer model, but the NN forward model is used in the retrieval algorithm." – Please explain the significance/advantage of this approach.

We prefer to use the synthetic data directly computed by the radiative transfer model to capture any difference between the radiative transfer simulation and the NN models. As shown in Eq (5), the contribution of the NN uncertainties has been considered in the total uncertainty model. We have added the following discussions:

"The synthetic data is computed directly using the vector radiative transfer model, but the NN forward model is used in the retrieval algorithm to achieve maximum efficiency. In this way the contribution of the NN uncertainties is captured both in the simulation and the uncertainty model as shown in Eq. 5. "

• Line 415: "retrieval algorithms can be further improved, for instance, by including additional a priori constraints" – what kind of constraints? – please be more specific.

Multiple constraints can be added as summarized in Dubovik et al 2021. For example, there could be smoothness constraints on the refractive index spectra, volume distribution, vertical profile etc. We have revised the sentence as:

> "The large ratios of real and theoretical uncertainties also indicate where retrieval algorithms can be further improved, for instance, by including additional a priori constraints, **such as smoothness in refractive index spectra and size distribution, temporal and spatial variations of the retrieval parameters. Various constraints in the framework of multi-term least square method are summarized by Dubovik et al., (2021)."**

• "Less number of measurements are" → "A smaller number of measurements is"
Updated.

• Line 440: "Higher measurements are generally" → '' A larger number of measurements is generally"
Updated.

• Line 450: "makes retrieval cost more uniform" – not clear, please rewrite.
Since the cirrus cloud angles are removed, the cost function appear more uniform across the scene. We have revised the sentence as follows

> "The χ^2map (shown in Gao et al 2021) shows that excluding the cirrus-contaminated angles makes retrieval **cost function more spatially uniform** across the scene."

• 495: "a more complicated ocean bio-optical model" → "a more complete and realistic ocean bio-optical model"
Updated

Technical Corrections
In general this paper is well written, and I did not spot any typographical or grammar mistakes, except for the following:
• Line 204: "explicit a prior information" → "explicit a priori information"
Updated

• Line 206: "we assume Sa" → "we assume **S**a"
Updated

• Line 207: "assumed a prior " → "assumed a priori"
Updated

• Line 329: “Rrs” → “*Rrs*”
Updated, also checked the whole document.

• Line 337: “their difference are quantified” → “their difference is quantified”
Updated

• Line 405: “errors are found sufficiently to evaluate” → ‘errors are found sufficient to evaluate”
Updated

• Line 518: “based on a high-cost function” → “based on a failure to properly minimize the cost function”
Thank you for the suggestion. We revised the statement slightly as follows:

> “Fewer suitable measurements tend to lead to larger retrieval uncertainty, although this is arguably preferable (considering data coverage) to **discarding the whole retrieval based on a high-cost function value.**”

Reference

Fan, Y., W. Li, N. Chen, J.-H. Ahn, Y.-J. Park, S. Kratzer, T. Schroeder, J. Ishizaka, R. Chang, and K. Stamnes, OC-SMART: A machine learning based data analysis platform for satellite ocean color sensors, Remote Sensing of the Environment, 253, 112236, 2021.