Response to the reviewers: Analysis of cloud fraction adjustment to aerosols and its dependence on meteorological controls using explainable machine learning # EGUSPHERE-2023-1667

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We would like to thank the two anonymous referees for reviewing the manuscript and providing very helpful and constructive comments. The reviewers' comments and suggestions are incorporated in italics and addressed hereafter and the authors' responses are colored in blue. If not explicitly stated otherwise, line numbers in this letter refer to the original manuscript (before the update). We have also added: "We thank two anonymous reviewers whose helpful comments contributed to improving the

5 manuscript." to the acknowledgements.

Referee 1

General comments

This is an interesting work focused on factors influencing the cloud fraction by using explainable machine learning approaches. The data and method are both solid, and the paper is well-written. I just found several places that need to be justified or

10 *clarified. Therefore, I recommend a minor revision for this paper to be published on ACP.* Thank you for the positive evaluation of the manuscript. Specific comments are addressed individually as follows.

Specific comments

Line 90: Does re means CLF? How cloud temperature, solar zenith viewing angle, and satellite zenith angle are used to filter and compute Nd?

15 r_e refers to cloud droplet effective radius (Section 1 Line 41). How cloud temperature, solar zenith viewing angle and satellite zenith angle are used to filter N_d is described from line 105 to Line 109. To clarify, we rephrased the sentence "Except for CLF ... and compute N_d " in Line 90 as "CLF serves as the predictand in this study. The computation of N_d relies on τ_c and r_e , with filtering criteria based on CTT, solar zenith viewing angle and satellite zenith angle, as elaborated in the following."

Line 110: How the reanalysis data are harmonized? Could you please provide a little more details, which spatial averaging

20 (interpolation) techniques have been used?

We have revised the related sentence at Line 111-112 with a more detailed description: "The ERA5 data sets are harmonized to fit the level-3 MODIS data by first being resampled to $1^{\circ} \times 1^{\circ}$ from their default $0.25^{\circ} \times 0.25^{\circ}$ spatial resolution using bilinear

interpolation, and they are subsequently collocated to Terra MODIS by extracting hourly data to align with the UTC overpass times of the Terra satellite for each grid cell, yielding a spatiotemporally matched MODIS-ERA5 combined data set for training

25 the ML models."

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Line 114: Why use 99 percentiles as the threshold? How extreme values will influence your interpretation of the ML model? We refined the sentences in Line 114 to explain this: "For N_d retrievals, only samples within 1–99 percentiles are retained to exclude potential unrealistic outliers from r_e and τ_c retrievals (Zipfel et al., 2022). Furthermore, the explanation of ML models in this study relies on using linear regressions to capture the distribution of individual prediction instances, and the

30 extreme values may excessively magnify or reduce the sensitivity or interactive effects quantified by SHAP (shown in Fig. 1 and discussed in Sect. 2.3.2). The threshold of 1–99 percentiles for each predictor is thus adopted to remove the values at the very tails of the specific distribution and to improve the robustness of the estimated sensitivities."

Line 136: 6000 data points as the threshold, would you please provide an estimate for the percentage of data dropped from the total sample?

- Thanks for the comment. The threshold of 6000 is used to guarantee that each $5^{\circ} \times 5^{\circ}$ "geographical window" has a sufficient volume of data to train and test the XGB models. As this study explicitly focuses on MBLCs, the $5^{\circ} \times 5^{\circ}$ windows encompassing continental or coastal regions and containing fewer than 6000 valid samples are not considered as "filtered out". For windows covering only oceans, 34 of them have fewer than valid 6000 samples due to the screening for N_d retrievals. These specific windows, located between 47.5°W–122.5°E and 52.5°S–57.5°S, have been consequently removed.
- 40 We have modified the corresponding statement to further clarify this: "To ensure a sufficient data amount for training and testing the XGB models, only the geographical windows with over 6000 available data points are retained. Consequently, 34 out of 1190 oceanic windows have been excluded. These windows located between 47.5°W–122.5°E and 52.5°S–57.5°S in the Southern Ocean (Fig. 2) contain fewer than 6000 valid samples due to the screening for N_d retrievals."

Line 180: The definition of IAI may need to be clarified, is it a slope or difference? how the difference is calculated, which minus which?

Thanks for the suggestion, the sentence has been revised for improved clarity as follows: "An interaction index (IAI) is derived from these regression fits and defined as the slope for the high-value group (> mean) minus the slope for the low-value group (< mean):

$$IAI = \beta_{x,high} - \beta_{x,low} \tag{2}$$

50 where β is the slope of the linear regression between SHAP interaction values and ln N_d values, and the subscripts denote the high-value group and the low-value group for a specific meteorological variable x (SST in the example), respectively. At the exemplary geographical window, the influence of SST on N_d -CLF sensitivity is quantified by IAI = -0.029 CLF σ^{-1} (Fig. 1 (b)). Similar to sensitivities, the unit of IAIs is also CLF σ^{-1} ."

Line 214: How do you explain that the PF is influencing the CLF but not vice versa? Same for some other predictors in the ML model.

For PF, we intended to use the ML framework in this study to represent the role of large-scale precipitation on MBLC ACIs. As theoretical knowledge suggests atmospheric aerosols tend to affect cloud properties differently for precipitating clouds (precipitation suppression) and non-precipitating clouds (enhanced entrainment feedbacks) as outlined in the introduction section. It was assumed that the setup of IAI would be able to capture these effects.

- 60 Yes, CLF could also exert an influence on PF and other predictor parameters, and there may be relevant feedback loops at play. Similar to PF, the selection of all predictors, which could be potentially recognized as main drivers within the context of ACI, is based on the literature and existing knowledge for better interpretability of causality. The sensitivities and meteorological influences on ACI quantified by SHAP regression values are statistically representative of physical processes at regional and daily scales. Nevertheless, it is important to note that the causal chain quantified by SHAP values in the ML models may not
- 65 necessarily reflect real-world physical causality, though this is an inherent and common limitation for all statistical analyses.We have added relevant discussions to the manuscript and rephrased it accordingly:
 - P. 7 L. 165: "SHAP values provide insights into the behaviour of the XGB models, and as all statistical/ML models, they may not necessarily reflect real-world physical causality. Nevertheless, this state-of-the-art technique allows us to account for meteorological covariations when deriving sensitivities and to appraise to what extent the meteorological predictors interact with and influence the N_d -CLF relationship beyond traditional global-level feature attributions."
 - P. 16 L. 352: "It should be noted ... N_d retrieval biases as a function of CLF. This would potentially contribute to the non-causal facets of the relationships and interactive effects quantified by SHAP values."

Line 229, SHF, please declare the full name of the acronym when it first appears in the text, even if it has been listed in table 1. Thanks for pointing it out, done. Full spellings of acronyms of other predictors have also been added when they are initially introduced in the main text. The use of full names and acronyms of all predictors has also been adjusted accordingly throughout

the manuscript.

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Section 3.3.2, Fig. 8, why RH850 is omitted? It shows higher importance than SST in Fig.7.

We want to emphasize the significance of EIS and SST, as they are critical components of the low-cloud feedback. RH can be regarded as an intermediate predictor as it can act as a proxy for various physical processes. The regional pattern of IAI for

80 RH_{850} is shown in Fig. 1 of this letter, in spite of the distinct patterns, the assertion of direct causality is challenging as relative humidity is linked to many meteorological processes.



Figure 1. Patterns of the Interaction Index showing the dependence of the N_d -CLF relationship on relative humidity at 850 hPa (RH₈₅₀).

Referee 2

General comments

This manuscript fits xgboost models to capture daily cloud fraction at 5x5 degree scale. They apply the SHAP calculation and

85 present results mostly in terms of the SHAP values and their variations to different values by holding individual variables out from model calculations. The authors argue that the results represent a 'better quantification of the responses of MBLC CLF to aerosols'. The topic is relevant for ACP. However, there are a few major methodological concerns I have and they are detailed in the following. In my opinion, they must be addressed before the paper can be published.

We thank the referee for the comments which are very helpful in making the manuscript clearer. The concerns are addressed 90 individually as follows:

Specific comments

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1. It is unclear what data constitute MBL CLF. Only daily MODIS level-3 data are mentioned, but AFAIK, MODIS daily data do not have a field called MBL CLF. The authors need to be clear on this.

We have made the relevant statement clearer on P. 3 L. 88–90: "In this study, MBLCs are defined as single-layer warm cloud fields with cloud top temperatures higher than 268 K. To achieve this, the information on CLF (product: Cloud_Retrieval_Fraction

_1L_Liquid_Mean), cloud top temperature (CTT; product: Cloud_Top_Temperature_Mean) and satellite viewing geometry are obtained from MODIS level-3 collection-6.1 atmosphere daily products on the Terra platform (MOD08_D3), which are gridded into $1^{\circ} \times 1^{\circ}$ globally from level-2 atmospheric products."

100 2. It is unclear how the data is standardized. The standardization procedure is easy to understand, but is this done globally or locally for each 5x5 box?

Standardization is done for each $5^{\circ} \times 5^{\circ}$ box before the training of each XGB model. We have added the information to the sentence on P. 4 L. 118 to clarify this: "All input data for each XGB model (i.e. for each $5^{\circ} \times 5^{\circ}$ window) are standardized for comparability of the estimates of the sensitivity and the interactive effect with meteorology (Sect. 2.3.2)."

- 105 3. Some inappropriate reference citing is noted. For example, line 37, 'Furthermore, MBLCs are especially susceptible to aerosol perturbations due to their physical properties (Wood et al., 2015).' This is a very vague and general statement with a field campaign overview paper as a reference. As a researcher working on this topic for a long time, I cannot follow what is being said or cited here. Line 45: these two references are relevant, but they are neither the earliest nor the best papers that explain the mechanism mentioned here. Line 50: Yuan et al., 2011 showed increase of cloud fraction with aerosols in the trade
- 110 cumulus region. Line 52: observational evidence of GCM overestimation of LWP adjustment was presented convincingly in Toll et al., 2019. Line 102: potential retrieval biases are extensively discussed in Zhang et al., 2011. Grosvenor et al 2018 has relevant info, but it is not specifically for this subject.

We thank the referee for bringing our attention to the references mentioned.

- Line 37: We agree that the choice of citing Wood et al. (2015) may not be the most suitable in this context. The sentence
- has been refined for better clarity and precision regarding "their physical properties". It has been altered as follows: "Furthermore, MBLCs are especially susceptible to aerosol perturbations due to their relatively low optical depths (Turner, 2007; Leahy et al., 2012) and their formation in environments typically characterized by lower anthropogenic aerosol loading than continental clouds (Platnick and Twomey, 1994)"
- Line 45: Thanks for pointing this out. We have updated the references in question and included sedimentation-entrainment
 feedback which can also lead to a decrease in clouds from increased N_d: "This has been found in particular for non-precipitating clouds, stemming from enhanced entrainment mixing with ambient air over the clouds owing to shorter evaporation timescales (Wang et al., 2003; Jiang et al., 2006; Small et al., 2009) or reduced sedimentation (Ackerman et al., 2004; Bretherton et al., 2007) because of smaller droplet sizes."

- 125 Line 52: We have added the suggested reference to Line 54 and rephrased the existing sentence: "This is supported by observational evidence presented by Toll et al. (2019) who also reported an overestimation of LWP adjustment in climate models, and by Chen et al. (2022) who recently highlighted the role of CLF increases due to aerosols from a large volcano eruption as the main cause of the associated forcing."
- Line 103: Thanks for pointing us to the earlier reference that discusses the potential r_e retrieval biases in heterogeneous clouds. We now cite Zhang and Platnick (2011) and Zhang et al. (2012) in the updated version of the manuscript: "In such heterogeneous cloud fields, subpixel effects in the retrieval of r_e can negatively bias the retrieved N_d values (Zhang and Platnick, 2011; Zhang et al., 2012; Grosvenor et al., 2018)."

⁻ Line 50: Thanks for the suggestion. Yuan et al. (2011) has been added to the manuscript.

4. SHAP values, as the authors corrected noted, are only ONE way of attempting to explain the boosted tree models. For each data point, there is a SHAP value for each explaining variable. By construct, they are 'situationally' dependent. They don't

- 135 really provide any physical insights. All the algorithm is trying to do is gradient boosting its model to best fit the data. In fact, the first figure shows that the way the authors try to use SHAP values to 'explain' results is not physical. Figure 1a shows that SHAP value for Nd generally gets larger with increasing Nd. Physically, it says that when clouds are more polluted, cloud fraction tend to increase with Nd more stronger. This runs against our physical understanding. Fitting a slope for the SHAP values and claiming this shows sensitivity of CLF to Nd are not valid IMO. I'd love to hear the authors' rationale here.
- 140 We agree with the reviewer that SHAP values are just one way of explaining tree-based machine learning (ML) models, in fact, many of these methods are related. SHAP values are basically the partial dependence of y on X_i but additionally include interactive effects for more complex models (as used here). These interactive effects make them 'situationally' dependent, which we exploit in our study. While we acknowledge that SHAP values provide insights into the behaviour of XGB models and do not necessarily reflect physical relationships, this limitation is true for any observational study that uses statistical/ML
- 145 methods to try and better understand physical processes. It should be noted though that SHAP values are a well-established and state-of-the-art method to get insights on processes from observational data in ML frameworks (e.g. Lundberg et al., 2020; Stirnberg et al., 2021; Zipfel et al., 2022; Li et al., 2022). Relevant discussions have already been added to the manuscript and the existing text has been rephrased accordingly:

P. 7 L. 165: "SHAP values provide insights into the behaviour of the XGB models, and as all statistical/ML models,
 they may not necessarily reflect real-world physical causality. Nevertheless, this state-of-the-art technique allows us to account for meteorological covariations when deriving sensitivities and to appraise to what extent the meteorological predictors interact with and influence the N_d-CLF relationship beyond traditional global-level feature attributions."

- P. 16 L. 352: "It should be noted ... N_d retrieval biases as a function of CLF. This would potentially contribute to the non-causal facets of the relationships and interactive effects quantified by SHAP values."
- Of course, we also agree with the reviewer that the ML model used just tries to best fit the data, but again, this is essentially true for any predictive statistical or ML model. It is just different mechanisms of fitting to the data that make them different. As such, we don't feel this is a valid criticism of using this method in this context.

We believe there is a misunderstanding with respect to the physical interpretation of the SHAP values for deriving the CLF sensitivities and the example of Fig. 1 (a) of the manuscript. "Physically, it says that when clouds are more polluted, cloud fraction tend to increase with Nd more stronger." This interpretation is not correct. The figure does show that the *contribution* of ln N_d to the prediction of cloud fraction scales with ln N_d , which is of course also the case in a linear model (Y = mX + b). In fact, in a linear model, SHAP values are just the difference between the base value (average value) and the predicted y (see Fig. 2 of this letter, left panel). Positive (negative) SHAP values indicate that the specific feature value increases (decreases) the prediction compared to this base value. In other words, the base value is the reference point against which the contributions

165 of individual features are measured, and the measure is SHAP values. If we designate this "reference point" as the zero point on the y-axis (subtracting the base value), we will get the y-axis in the right panel. In the case of a linear regression, the slopes



Figure 2. Figures taken from the SHAP documentation page, section "An introduction to explainable AI with Shapley values" on: https://shap.readthedocs.io/en/latest/overviews.html, last accessed 22 October 2023.

of regression models fit to the original data and the SHAP values are equal, it is just that the intercept of the line changes by the base value (as if the y-axis were shifted by the base value, cf. Fig. 2). As such, it is clearly valid to fit a line to SHAP values and interpret the slope as the sensitivity of y to X_i , and this is also the reason why the derived sensitivity patterns are so similar compared to the other satellite-based studies cited in the manuscript.

Figure 1 (a) of the manuscript illustrates that - in the considered geographical window - as $\ln N_d$ increases, the SHAP values for $\ln N_d$ consistently increase (see the dashed line). Hence, the correct physical interpretation of Fig. 1 (a) within the manuscript is that as clouds become more polluted, the predicted CLF exhibits a nearly linear increase. which is in agreement with our physical understanding. The advantage of this method is twofold: 1) meteorological covariates are considered in the quantification of SHAP values and thus accounted for in the derived sensitivities, 2) possible effects of 3rd variables on the

175 quantification of SHAP values and thus accounted for in the derived sensitivities, 2) possible effects of 3rd variables on the N_d -CLF relationship can be analyzed with interactive effects.

To make the manuscript clearer, we also have expanded and provided a more comprehensive explanation of SHAP values on P. 7, L. 155–157: "The base value in the context of SHAP values is typically computed as the average of all predictions by ML models over the entire training data points. Positive (negative) SHAP values indicate that the specific feature value increases

180 (decreases) the prediction compared to this base value. In other words, the base value serves as the reference point against which the contributions of individual features are measured. SHAP values for all features will always sum up to the difference between the base value and the final model prediction so that SHAP values are additive and internally consistent."

5. What follows in the manuscript is thus questionable. I will reserve my comments for the next version after the authors address the important methodological question.

185 We believe that the questions and comments have been properly addressed.

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Minor modifications independent of the reviewer comments

- P. 3 L. 79: "SHAP" appears for the first time in the main text, the full spelling has been added here.
- P. 4 L. 97: The blank between 50 and % has been deleted.
- P. 4 L. 110: "20" has been removed from the text.
- 190 P. 6 L. 152: Addition reference (Li et al., 2022) has been added.

P. 7 L. 159: "when" is added between "versus" and "it".

P. 7 L. 172: "isolated" is now removed from the text.

P. 7 L. 173: the unit of the sensitivity (CLF σ^{-1}) has been added after 0.098. The sentence originally in L. 184 "Note that all the input data have been standardized ... standard deviation (CLF σ^{-1})." has been restructured and split into L. 174 and L. 181,

- 195 respectively, after mentioning the values of sensitivities and IAIs in the example. P. 8 Figure 1: We added the unit of the sensitivity and IAI (CLF σ^{-1}) to the legends of subplots.
 - P. 11 L. 238: "Sec. 2.1" to "Sect. 2.1"

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