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Key Points:

- Cloud phase in polar regions can be predicted based on cloud top temperature, sea ice concentration, and sea salt and dust mixing ratios
- Cloud top temperature has the strongest impact, while sea salt/spray aerosol is relevant for low-level, and dust for mid-level cloud phase
- Sea ice coverage and Southern Ocean westerly winds may influence the aerosol distribution and thereby cloud phase

Supporting Information:

Supporting Information may be found in the online version of this article.

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Combined Impacts of Temperature, Sea Ice Coverage, and Mixing Ratios of Sea Spray and Dust on Cloud Phase Over the Arctic and Southern Oceans

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Abstract We analyze the importance of cloud top temperature, dust aerosol, sea salt aerosol, and sea ice cover for the thermodynamic phase of low-level, mid-level, and mid to low-level clouds observed by CloudSat/CALIPSO over the Arctic and the Southern Ocean using an explainable machine learning technique. As expected, the cloud top temperature is found to be the most important parameter for determining cloud phase. The results show also a predictive power of sea salt and sea ice on the phase of low-level clouds, while in mid-level clouds dust shows predictive power. Over the Southern Ocean, strong zonal winds coincide with the aerosol distribution. While they can produce high mixing ratios of sea spray at lower levels, the strong zonal winds may prevent the pole-ward transport of dust. Sea ice may prevent the release of sea salt aerosols and marine organic aerosols leading to higher liquid fractions in clouds over sea ice.

Plain Language Summary The cloud phase describes whether a cloud consists of ice particles, liquid droplets, or both. The representation of the cloud phase in climate and weather models is uncertain, leading to radiation biases over the Southern Ocean and the Arctic Ocean. To investigate the impact of four different parameters on the cloud phase, we use an explainable machine learning technique. The parameters studied are the temperature of the cloud top, the sea ice coverage, and the concentration of sea salt aerosols and dust aerosols, both of which can act as ice nucleating particles and contribute to the ice formation in clouds. We find that temperature seems to be the most important factor in determining the cloud phase. Sea salt aerosol seems to be more relevant for low-level clouds closer to the ocean surface, the source of sea salt aerosol. Sea ice may prevent the release of sea salt aerosol by covering the ocean and our analysis supports this hypothesis. Dust is typically transported over long distances and our analysis shows that dust aerosol is more important for mid-level clouds, but persistent strong winds surrounding Antarctica may have an influence on the dust concentration and thus on cloud phase.

1. Introduction

The uncertainty of the representation of cloud phase over the Arctic and the Southern Oceans leads to radiative biases in climate and weather models. The latest iteration 6 of the Coupled Model Intercomparison Project (CMIP6) shows a large intermodel spread of the representation of clouds globally, but especially in low and middle heights over polar regions (Cesana et al., 2022). The long-standing shortwave radiative bias over the Southern Ocean has been slightly improved in CMIP6 simulations compared to previous versions, but the multimodel mean bias of the shortwave cloud radiative effects is still up to 18 Wm^{-2} zonally averaged south of 55°S, while it is negative north of 55°S (Cesana et al., 2022). Over the Arctic, CMIP5 simulations also showed large uncertainties in the representation of low-level clouds (Taylor et al., 2019), and CMIP6 shows mostly an overestimation of the cloud fraction (Wei et al., 2021) also leading to radiative biases. Besides climate models, weather simulations also show uncertainties and biases in the representation of clouds over the Arctic (Klein et al., 2009; McCusker et al., 2023; Solomon et al., 2023; Tjernström et al., 2021). To improve the representation of cloud phase over the Arctic Ocean and the Southern Ocean, an improved understanding of the factors influencing cloud phase is needed. In addition to meteorological factors, dust has been identified to co-vary with cloud glaciation (Kawamoto et al., 2020; Villanueva et al., 2020). Our previous analysis (Dietel, Sourdeval, & Hoose, 2024) has shown that aerosol correlations with the thermodynamic phase of low-base and mid-base clouds

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are largest for dust and sea salt over the Arctic and Southern Ocean. While dust is a known type of ice nucleating particle, sea salt over the polar oceans is often co-emitted with organic materials from the ocean micro-layer, resulting in sea spray aerosols, which can nucleate ice at high temperatures (Burrows et al., 2013; DeMott et al., 2016; Ickes et al., 2020; McCluskey et al., 2018; Wilson et al., 2015). Besides aerosol correlations with cloud phase, sea ice also showed correlations with cloud phase (Carlsen & David, 2022; Dietel, Sourdeval, & Hoose, 2024). However, it is not yet clear how different factors influencing cloud phase interact, how large their respective contributions to cloud phase are, and how their impact varies regionally.

In this study, we quantify the impact of cloud top temperature, sea ice concentration, dust, and sea salt for cloud phase by analyzing satellite observations and reanalysis data in an explainable machine learning framework. We consider sea salt in this study as a proxy for sea spray aerosols including co-emitted organic INPs. We also investigate the regional distribution of the parameter influence on cloud phase. The machine learning method allows to untangle the effects of the influencing factors of cloud phase.

2. Data

A detailed description of the data set used can be found in Dietel, Sourdeval, and Hoose (2024), but we will summarize the most important information in the following.

This study is based on a 2-year data set (2007 and 2008) of cloud phase information from DARDAR (Delanoë & Hogan, 2008, 2010) over the Southern Ocean (40°S–82°S) and the Arctic Ocean (60°N–82°N) excluding data over land surfaces to reduce uncertainties introduced by orography. We analyze single-layer low-level, mid-level clouds, and mid-to-low-level clouds, henceforth mid-low-level which are defined by their cloud top height (CTH) and their cloud base height (CBH) as described in Dietel, Sourdeval, and Hoose (2024). Low-level clouds are defined as clouds with CBH and CTH between 0.5 and 2 km, mid-level clouds with a CBH and CTH larger than 2 km, but lower than a thresholds z linearly increasing from 4 km at the pole to 7 km at 40°S/N, and mid-low-level clouds are defined by a CBH between 0.5 and 2 km, and a CTH between 2 km and the mentioned threshold z. For each cloud profile, we calculate the liquid fraction (f) with Equation 1 based on the number of liquid vertical bins (n_{Liq}), mixed-phase vertical bins (n_{Mix}), and ice vertical bins (n_{Ice}). The factor 0.5 is used in absence of better information assuming half of a mixed-phase vertical bin consists of ice particles and half of it consists of liquid droplets. The results are not very sensitive to this choice (see Figure S1 in Supporting Information S1).

$$f = \frac{n_{\mathrm{Liq}} + 0.5 \cdot n_{\mathrm{Mix}}}{n_{\mathrm{Liq}} + n_{\mathrm{Mix}} + n_{\mathrm{Ice}}} \tag{1}$$

Collocated 3-hourly mixing ratios of dust and sea salt from the ECMWF Atmospheric Composition Reanalysis 4 (EAC4) (Inness et al., 2019) from the Copernicus Atmosphere Monitoring Service (CAMS) are used. The size modes are summed up and mixing ratios are averaged over the cloud heights for each cloud profile. The horizontal resolution of the aerosol data is about 80 km. In this study, sea salt is used as proxy for sea spray aerosols, including organic materials. Daily sea ice concentrations with a horizontal resolution of 25 km from Nimbus-7 SMMR and DMSP SSM/I-SSMIS Passive Microwave satellite instrument version 1 (Cavalieri et al., 1996) are also collocated to the cloud profiles. Cloud top temperature is derived from the temperature provided as part of the DARDAR data set coming from the ECMWF-AUXillary (ECMWF-AUX) product (CloudSat DPC, 2024).

3. Method of Explainable Machine Learning Technique

A Histogram-based Gradient Boosting Regression Tree model (based on the python package scikit-learn (Pedregosa et al., 2011)) is trained to predict the liquid fraction of a cloud using the four parameters of cloud top temperature, sea ice concentration below the cloud, dust aerosol mixing ratio, and sea salt aerosol mixing ratio. These are selected because our previous study (Dietel, Sourdeval, & Hoose, 2024) has shown correlations of the cloud phase with these parameters. Furthermore, it is known that a decreasing temperature leads to an increased freezing probability, while aerosols like dust and sea spray including marine organics can act as INP and thereby influence cloud phase. Sea ice cover changes surface conditions, but is also hypothesized to reduce sea spray emission and thereby indirectly influence cloud phase. Six different models are trained for the combinations of three different cloud types, low-level, mid-level, mid-low-level, over the two regions of the Southern Ocean and the Arctic Ocean. Due to different cloud type occurrence frequencies, the training sample sizes vary, but the

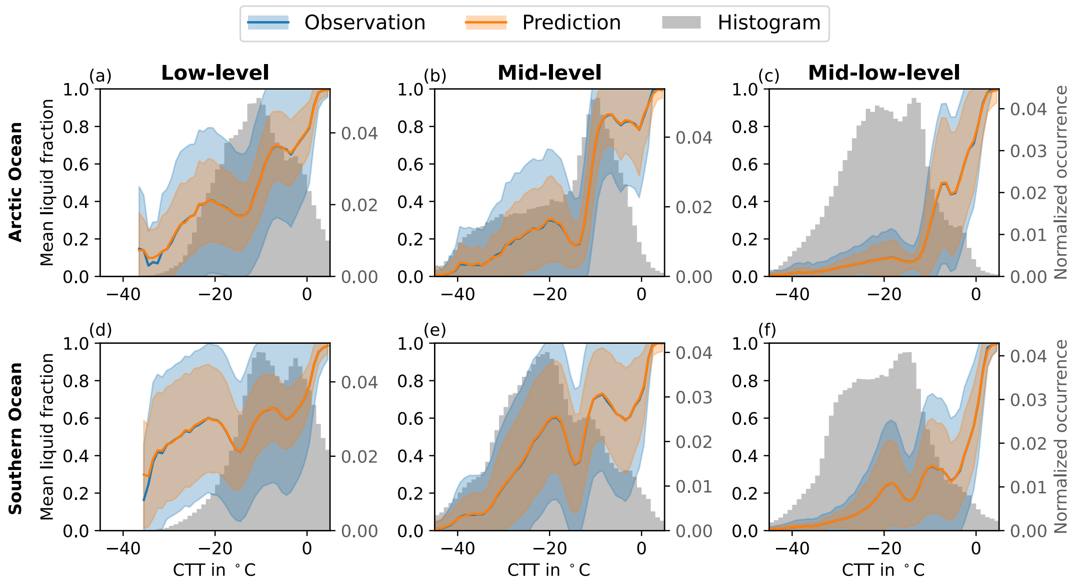

Figure 1. Mean of the observed liquid fraction as a function of cloud top temperatures (CTT) and mean of the liquid fraction predicted by the machine learning models with shaded areas representing standard deviations. The gray histogram shows the distribution of cloud top temperatures in the validation subset (500,000 samples).

smallest training sample size still has 300,000 samples (see Table S2 in Supporting Information S1). The training and validation data sets are randomly sampled subsets of the original data set. Being much faster than other Gradient Boosting Regressors, this machine learning model is well-suited for our purpose and large data sets, as the input samples are binned before the gradient boosting, which reduces the training for finding the optimal split (Tamim Kashifi & Ahmad, 2022). Furthermore, decision trees are well-suited for parameters covering different size ranges. We don't use spatial or temporal information for the model training, but use only the four feature parameters to predict the liquid fraction independent of the location and time.

After a manual testing of hyperparameters, a grid search method including a 3-fold cross validation (GridSearchCV from the python package scikit-learn) is used to find the optimal set of hyperparameters (see Table S1 in Supporting Information S1). To investigate the importance and influence of different parameters on the prediction, we use SHAP values (S. Lundberg & Lee, 2017; S. M. Lundberg et al., 2020) as a Tree Explainer method, which show the quantitative contribution of each feature value to the prediction. SHAP values show the marginal contribution of a feature to a prediction while considering all permutations of the feature values. Due to computational costs, we calculate them for a representative subset of 500,000 samples for each cloud type over each region. If two (or more) features co-vary, the SHAP values cannot separate the contributions of the features to the prediction, and might even give misleading results. However, as the size of the samples is very large, such that is likely that it contains sufficient independent variation. We also investigate the spatial distribution of the importance of the parameters compared to the averaged importance for the complete region of the Arctic Ocean or the Southern Ocean.

4. Results and Discussion

The models can predict the liquid fraction based on the feature variables. Figure 1 shows a good agreement between observations and predictions of the mean liquid fraction as a function of the cloud top temperature. The performance of the models is also shown by Pearson correlation coefficients between observations and predictions for the validation data set, which is in the range of 0.61 and 0.85 for different cloud types and regions (see Table S2 in Supporting Information S1).

4.1. Importance of Parameters for Cloud Phase

To assess the importance of the individual model features on cloud phase, we separate these into three groups of low (smaller than 25th percentile), middle (between 25th and 75th percentile), and high (larger than 75th percentile) feature values and analyze the distribution of SHAP values in these groups (Figure 2). For the sea ice

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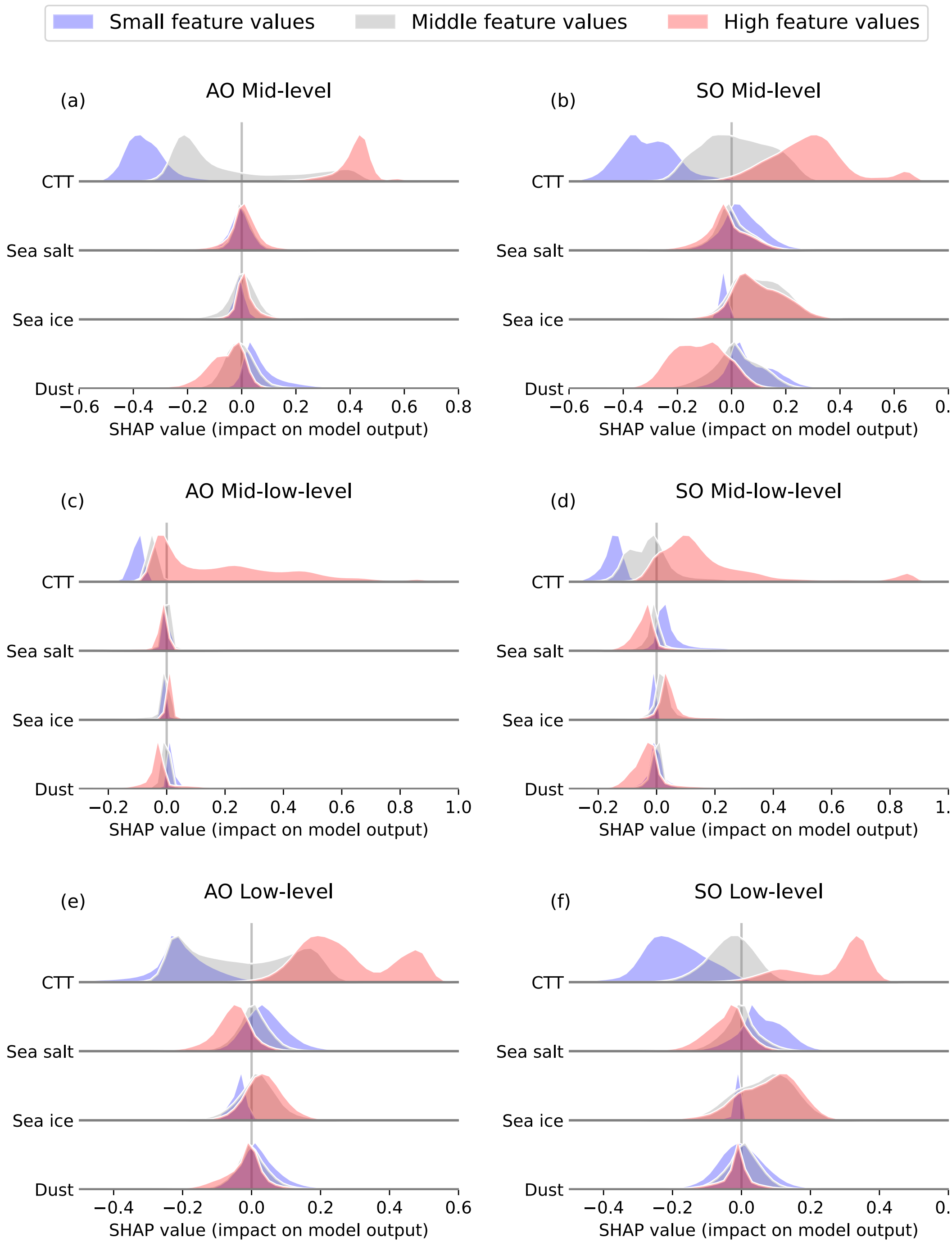

Figure 2. Distribution of SHAP values of different features, namely CTT, sea ice concentration, dust mixing ratio, and sea salt mixing ratio. The colors correspond to small ($X \leq P25$, blue), middle ($P25 < X \leq P75$, gray), and high ($P75 < X$, red) values, based on the 25th percentile ($P25$) and the 75th percentile ($P75$) of the feature values, except for sea ice. Small sea ice concentration refers to values of zero, middle sea ice concentration refers to values larger than 0 and lower or equal than 0.8, while high values refer to larger than 0.8. Each distribution represents a probability density function based on a density estimation using Gaussian kernels. Each distribution is scaled by the maximum value of the distribution to improve readability. Left column: Southern Ocean, right column: Arctic Ocean.

concentration the group division is not based on percentiles, because of the distribution, but low values correspond to a sea ice concentration of 0, middle values correspond to a sea ice concentration between 0 and 0.8, and high values correspond to a sea ice concentration larger than 0.8. All cloud types show the largest absolute SHAP

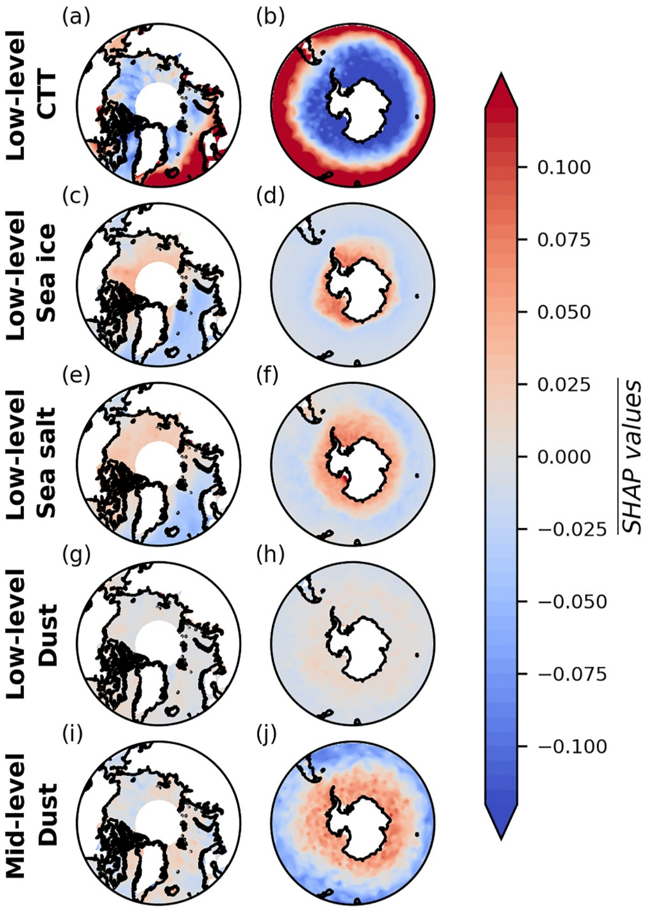

Figure 3. Regional distribution of the averaged SHAP values for different features, namely CTT, sea ice concentration, sea salt mixing ratio, and dust mixing ratio for low-level clouds and dust mixing ratio for mid-level clouds. Left column: Arctic Ocean, right column: Southern Ocean. Positive (negative) SHAP values (reddish (blueish)) refer to an increased (decreased) liquid fraction, based on the feature parameters CTT, Sea ice, Sea salt, and Dust. For the direction from the input parameter to the predictor see Figure 2.

values for the parameter of cloud top temperature with strongest differences of SHAP values between high and low cloud top temperatures. SHAP values of other parameters show smaller differences (Figure 2). Low temperatures correspond to negative SHAP values and a decreased predicted liquid fraction and vice versa. This highlights the importance of the temperature for cloud phase, which is expected as decreasing temperature leads to an increasing freezing probability. Besides temperature, the influence of the features varies between the cloud types. Dust shows a higher impact in mid-level clouds with higher dust concentrations leading to a lower liquid fraction (shown by negative SHAP values), which could be explained by dust acting as ice nucleating particles and thereby inducing ice formation (Hoose & Möhler, 2012). Sea salt is most relevant in low-level clouds over both polar regions and also shows a reduced liquid fraction for higher sea salt concentrations. This is in line with the fact that sea salt as a proxy for co-emitted marine organics (or sea spray) can also act as ice nucleating particles and thereby induce ice formation (Burrows et al., 2013; DeMott et al., 2016; Ickes et al., 2020; McCluskey et al., 2018; Wilson et al., 2015). Mid-level and mid-low-level clouds over the Southern Ocean also seem to be slightly impacted by sea salt. Low sea ice concentrations lead to a lower liquid fraction in low-level clouds over both regions and in mid-level clouds over the Southern Ocean, while other cloud types only show smaller influences by sea ice. It is hypothesized that sea ice prevents the release of sea spray leading to lower INP concentrations and thereby higher liquid fractions over sea ice. This will be further analyzed in the next section investigating the regional distribution of the impact of the different parameters on cloud phase.

4.2. Regional Distribution of Parameter Impact on Cloud Phase

The regional distribution of the influence of the different parameters on the model prediction shows a strong gradient in the SHAP values for cloud top temperature in low-level clouds (Figure 3). This is related to the general temperature gradient, which can also be seen in the cloud top temperature of low-level clouds (see Figure S2 in Supporting Information S1). Generally, the regional analysis shows strongest differences in the SHAP values for low-level clouds (see Figures S4 and S5 in Supporting Information S1). SHAP values of sea ice and sea salt show similar regional patterns. This also supports the hypothesis that there is a connection between sea ice coverage and the presence of sea spray influencing cloud phase. Regions where sea ice can occur show mostly positive SHAP values for sea salt representing higher predicted liquid fractions. Contrarily, SHAP values for sea salt are mostly negative in regions, where no sea ice occurs representing a reduced liquid fraction. We hypothesize that mixing ratios of sea salt and co-emitted organics are higher over the open ocean than over sea ice. The emitted sea spray can induce ice formation by acting as INP and thereby leads to lower liquid fractions in clouds over the open ocean compared to sea ice covered regions. Nevertheless, there may be dynamical processes connected to the presence of sea ice impacting cloud phase, which can be investigated in future studies. Dust shows only smaller SHAP values in low-level clouds compared to the other parameters. For mid-level and mid-low-level clouds cloud top temperatures also shows the largest absolute SHAP values in the regional analysis (see Figures S4 and S5 in Supporting Information S1). The other parameters show smaller SHAP values with less clear regional differences. While in Figure 2 dust shows an impact on the phase of mid-level clouds, Figure 3 shows that there is no consistent regional pattern of the influence of dust. This may be explained by temporally variable dust concentrations, which depend on long-range transport. This long-range transport of dust can have a strong effect on the phase of mid-level clouds, but is not connected to specific regions in the Arctic. Furthermore, other aerosol sources from land surfaces surrounding the Arctic like anthropogenic aerosols from factories may play a role and influence cloud phase, though they are not well represented in current reanalyses.

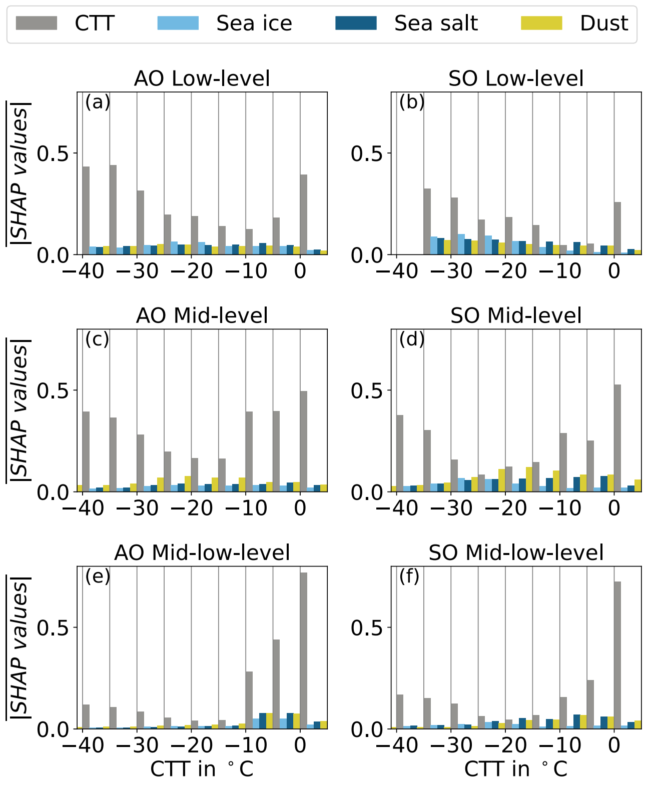

Figure 4. Mean absolute SHAP values of different feature parameters as a function of CTT for different cloud types over the Arctic Ocean (AO, left column) and the Southern Ocean (SO, right column). Four bars always correspond to the same 5°C bin, which is indicated by the small grid lines.

Contrarily to the Arctic Ocean, the regional distribution of the SHAP values over the Southern Ocean show a much stronger meridional gradient in most patterns. The SHAP values of the cloud top temperature of low-level clouds show the strongest meridional gradient, probably related to the strong zonal winds at the polar front surrounding Antarctica, and the Antarctic Circumpolar Current (ACC). SHAP values of sea ice show strong positive values in regions where sea ice occurs, while in other regions the values are mostly negative. The presence of sea ice leads to a higher liquid fraction in the model prediction. The pattern of the SHAP values of sea ice again correlates with the pattern of SHAP values of sea salt, similar to the Arctic Ocean, but sea salt production also depends on other factors like surface wind velocity. Nevertheless, we can see a reduced prediction of the liquid fraction due to sea salt (used as a proxy for co-emitted INPs) in regions where the ocean is usually not covered by sea ice and therefore sea spray concentrations are higher compared to regions covered by sea ice. SHAP values of dust are lower in low-level clouds, but larger in mid-level clouds with a strong meridional gradient with more positive values pole-ward. Figure 2 shows that high dust mixing ratios correspond with negative SHAP values and a decreasing liquid fraction, while low dust concentrations show more positive SHAP values and an increasing liquid fraction, which corresponds to the knowledge of dust acting as ice nucleating particle and contributing to ice formation. The strong meridional gradient can also be seen in the mixing ratio of dust (see Figure S3 in Supporting Information S1), and may also be related to the strong zonal winds, preventing the pole-ward transport of dust to high southern latitudes (Li et al., 2008). This effect is contrary to the usual temperature gradient and might at least to some degree counteract the influence of temperature on cloud phase. In mid-low-level clouds, the largest absolute SHAP values are shown for CTT, but small impacts of sea ice and sea salt can be seen again correlating spatially (see Figure S4 in Supporting Information S1).

4.3. Impact of Feature Parameters as a Function of Cloud Top Temperature

Besides the regional distribution, the relative impact (given by the SHAP values) of the different features as a function of cloud top temperatures (Figure 4) is of interest, as many models parameterize the cloud phase based on

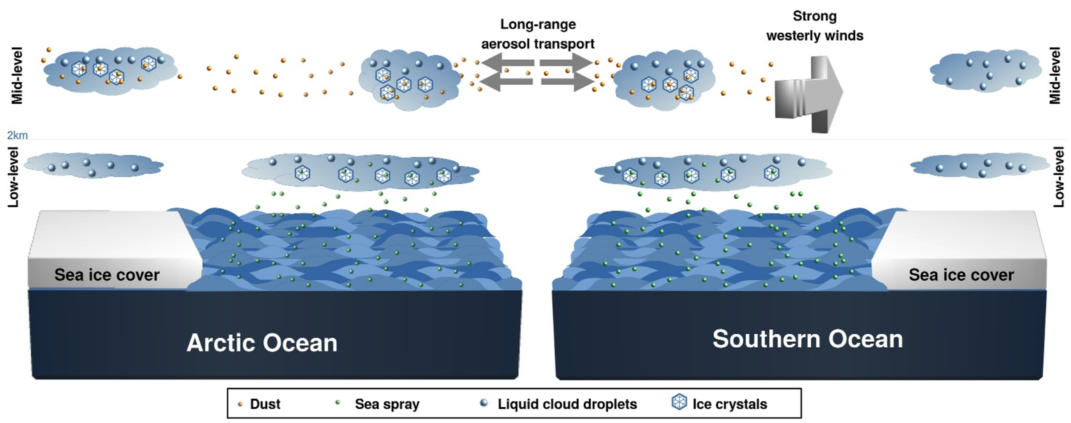

Figure 5. Summary schematic of possible parameters (in addition to temperature) influencing the phase of low-level and mid-level clouds over the Arctic and the Southern Ocean. Low-level clouds over sea ice show higher liquid fractions compared to low-level clouds over open ocean. This is hypothesized to be related to the emission of sea spray aerosol with co-emitted INPs, which is prevented by sea ice cover, leading to fewer INPs over sea ice. Mid-level clouds seem to be more affected by other long-range transported aerosol types like dust acting as INPs. Over the Southern Ocean, the pole-ward transport of dust seems to be blocked by strong westerly winds, leading to higher liquid fractions in mid-level clouds at high latitudes, possibly due to fewer INPs.

temperature. The impact of temperature becomes stronger toward the edges of the mixed-phase temperature regime, where the relative impact of other parameters decreases, as expected when the droplets remain liquid at/above 0°C or freeze homogeneously below −38°C. The SHAP values of the other parameters are more constant with temperature with the notable exception of dust in mid-level clouds, which has a maximum impact at CTTs of about −20°C. Further analysis (Figures S6–S9 in Supporting Information S1) revealed that this signal shows little seasonal variation over the Southern Ocean, but is strongest in winter over the Arctic Ocean. Over the Southern Ocean, the SHAP values for dust are even similarly high as the SHAP values for temperature in this intermediate CTT range. In low-level clouds sea ice and sea salt (as a proxy for co-emitted INPs) are the second most important parameters in most parts of the mixed-phase temperature regime. As the mean SHAP values for the aerosol variables and sea ice mostly do not show a strong temperature dependence, temperature-dependent aerosol properties are probably not the cause of the non-monotonous behavior of the liquid fraction (Figure 1), which are not well understood (Dietel, Sourdeval, & Hoose, 2024).

5. Conclusion

Using a histogram-based gradient boosting regression model and SHAP values as an explainable machine learning technique, we showed that temperature is the most important parameter determining cloud phase over the Arctic and the Southern Ocean. The impacts besides temperature are illustrated schematically in Figure 5 and show that sea salt (used as a proxy for sea spray) seems to be more relevant for low-level clouds phase, but correlates strongly with the impact of sea ice. This encourages the hypothesis that sea ice prevents the release of sea salt aerosol (Carlsen & David, 2022; Dietel, Sourdeval, & Hoose, 2024) leading to fewer INPs and therefore higher liquid fractions over sea ice compared to a cloud over open ocean with the same cloud top temperature. The role of dynamical processes and resulting microphysical regimes, for example, regarding secondary ice production, connected to the presence of sea ice can be a further reason of the impact of sea ice on cloud phase and should be investigated in future studies. Mid-level clouds phase seem to be more influenced by dust, while over the Southern Ocean a strong meridional gradient of its influence is observed. We hypothesize that the strong meridional winds inhibit the long-range transport of dust to high latitudes, leading to fewer INPs. Over the Arctic Ocean, there are no strong spatial/regional patterns of the influence of dust on cloud phase, and they are probably more dependent on current synoptic wind patterns, temporally varying. Furthermore, other aerosols from surrounding land sources may be more relevant over the Arctic Ocean than over the very remote Southern Ocean.

Data Availability Statement

The scripts to train the machine learning model used in this study is published in an institutional repository at https://doi.org/10.35097/VEbaqHtbXdEzreqO (Dietel, Andersen, et al., 2024). The DARDAR products (Ceccaldi et al., 2013; Delanoë & Hogan, 2008, 2010; Sourdeval et al., 2018) are provided by the Aeris/ICARE data center (https://www.icare.univ-lille.fr/dardar/). The sea ice concentration from Nimbus-7 SSMR and DMSP SSM/I-SSMIS Passive Microwave Data Version 1 (Cavalieri et al., 1996) are provided on the website of the National Snow and Ice Data Center (https://nsidc.org/data/nsidc-0051/versions/1). The aerosol mixing ratios from the CAMS reanalysis data (Inness et al., 2019) are available on the CAMS Atmosphere Data Store (ADS) website (https://ads.atmosphere.copernicus.eu/cdsapp#!/dataset/cams-global-reanalysis-eac4?tab=overview).

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