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IMPROVING OUR UNDERSTANDING OF CLOUD PHASE-PARTITIONING USING LONG-TERM CLOUD-RESOLVING SIMULATIONS OF SVALBARD

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Education and *justice* are democracy's only life insurance.

— Nannie Helen Burroughs

ABSTRACT

Clouds cover a large part of the Earth and are relevant for the hydrological cycle and the Earth's radiative budget. Clouds are very frequent in the Arctic, where they warm the surface most of the year in contrast to the rest of the globe. Low-level clouds are especially common in the Arctic and frequently contain supercooled liquid and frozen water simultaneously. The cloud's composition and radiative properties depend on the aerosols available for droplet or ice particle formation and the microphysical processes that drive the hydrometeor growth and interactions between the hydrometeors. Changes in the composition of clouds due to climate change can affect the cloud's radiative properties. Such changes can impact the larger climate system and amplify or dampen the warming. However, it is not fully clear what effect the changes in cloud properties and occurrence will have in the future. These uncertainties in models are due to several challenges, and one of the main ones is the representation of subgrid-scale microphysical processes in clouds. These processes, as well as the availability of aerosols, must be parameterised. These microphysical parameterisations inherit the knowledge gaps which still exist related to microphysical processes. With inaccurate parameterisations, models cannot correctly capture the radiative properties of clouds, and climate models can hardly quantify the impact of clouds in a warmer climate.

To address this issue, this thesis evaluates cloud-resolving simulations performed for a region of Svalbard, centred at Ny-Ålesund. Ny-Ålesund offers a variety of long-term measurements which are used as a reference. This location further provides a complex topography to challenge the model. As the chosen model was the ICON (ICOsahedral Nonhydrostatic) model, which was developed for Germany, the first goal is to evaluate the model's overall performance. It is shown that the model can capture large-scale features such as the wind flow and temperature profiles well. Compared to the observations, it also shows a similar cloud occurrence, but it is noticeable that there is an apparent underestimation of the mixed-phase clouds. It was further found that the liquid water path (LWP) is skewed towards higher values, so it became clear that the model glaciated clouds excessively. This misrepresentation of the cloud phase-partitioning has also been found in other models and was therefore further explored in the second study. The second study gave insights into whether the supercooled liquid representation would change using different aerosol settings. For this, the activation and nucleation schemes of

cloud condensation nuclei and ice nucleating particles were adjusted to fit the Arctic better, where the aerosol concentration is lower than in the mid-latitudes. This led to a substantial decrease in water droplets for the lower concentrations and increased raindrop concentrations. The LWP was further found to be better captured compared to the observations for lower LWP values. It seemed, though, that the lower aerosol numbers caused an over-correction of the LWP with no high LWP values for the new setup. Additionally, the change in the number of mixed-phase clouds was minor, indicating that the phase-changing microphysical processes potentially play a larger role in creating mixed-phase regimes.

To look further into the microphysical processes, a diagnostic tool was implemented that enables the output of the microphysical process rates. This tool was then used to explore which processes contribute most to the phase changes of hydrometeors. Here, it was found that there were clear differences between polar night and polar day, presumably to a large extent because of the temperature differences. Further, it became clear that phase changes via the vapour phase dominated and this also showed in the occurrence of the Wegener-Bergeron-Findeisen process, which could be quantified. To summarise, three main questions are addressed related to the performance of the ICON model in the Arctic, the impact of aerosols on supercooled liquid, and the microphysical processes contributing to phase changes. Combining all results, the picture emerged that substantial improvements in the representation of the phase-partitioning of clouds, especially low-level clouds, are necessary in ICON. These improvements can only be achieved by looking at both the aerosols and the microphysical processes. A better understanding of which mechanisms in models play a role in determining cloud properties has been achieved through the thorough investigation of long-term cloud-resolving simulations and the cloud microphysical processes. The methodological approach of using a large simulation data set, in combination with the implementation of a diagnostic tool, can be used in future studies and enables an increased understanding of why models behave in certain ways.

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ACRONYMS

AA Arctic Amplification

ABL Atmospheric Boundary Layer

AWIPEV German-French research base in Ny-Ålesund, Svalbard

CCN Cloud Condensation Nuclei

CMIP Coupled Model Intercomparison Project

CRE Cloud Radiative Effect

DNS Direct Numerical Simulation

ECS Effective Climate Sensitivity

GCM General Circulation Model or Global Climate Model

GLOBE The Global Land One-kilometer Base Elevation

Hande CCN CCN activation scheme by Hande et al. (2016)

Hande INP INP nucleation scheme by Hande et al. (2015)

HATPRO Humidity and Temperature PROfiler

ICON ICOsahedral Non-hydrostatic model

IN Ice Nuclei

INP Ice Nucleating Particle

IQR InterQuartile Range

IWP Ice Water Path

IWV Integrated Water Vapour

LEM Large-Eddy Model

LES Large-Eddy Simulation

LLC Low-Level Cloud

LW Longwave

LWP Liquid Water Path

MERIT-DEM Multi-Error-Removed Improved-Terrain Digital Elevation Model

ML Machine Learning

MPC Mixed-Phase Cloud

MWR MicroWave Radiometer

NWP Numerical Weather Prediction

PAMTRA Passive and Active Microwave TRAnsfer forward model

Phillips INP nucleation scheme by Phillips, DeMott, and Andronache (2008)

PSD	Particle Size Distribution
RANS	Raynolds-Averaged Navier-Stokes
SB06	2-moment microphysics scheme by Seifert and Beheng (2006)
SK	CCN activation scheme by Segal and Khain (2006)
SW	Shortwave
SLF	Supercooled Liquid Fraction
TOA	Top Of the Atmosphere
WBF	Wegener-Bergeron-Findeisen process

Part I

MOTIVATION & OBJECTIVES

1 WHY STUDY CLOUDS IN THE ARCTIC?

1.1 A WARMING ARCTIC

To begin with, focusing on the Arctic, it is necessary to explain the relevance of Arctic atmospheric research. By now, it is undeniable that the Earth is warming due to human-made emissions and that this has started to show in many locations around the globe, including the Arctic (IPCC, 2021). This rapid climate change is known to harm Earth's nature, including humans. In the Arctic, the warming is most visible from October to May (Figure 1, AMAP, 2021) and shows spacial inhomogeneities. The implications of the changing Arctic climate are not limited to the Arctic. The changes are also thought to impact the mid-latitude circulation, potentially causing an increase in extreme weather (Francis and Vavrus, 2012; Handorf et al., 2017). The warming of the Arctic is taking place faster than the average warming of the globe and is referred to as *Arctic Amplification* (AA). In several studies, the amplification factor was found to be around two to three (e.g. Bekryaev, Polyakov, and Alexeev, 2010; Druckenmiller et al., 2021; Walsh, 2014), but a recent study by Rantanen et al. (2022) suggests the warming could even be taking place four times as fast. The reasons for these discrepancies are mainly the difference in the definition of the Arctic region, the analysed period, and the data sources evaluated in the different studies. As discussed in Rantanen et al. (2022), current climate models tend to underestimate the Arctic amplification factor compared to past observations substantially.

"It is unequivocal that human influence has warmed the atmosphere, ocean and land. Widespread and rapid changes in the atmosphere, ocean, cryosphere and biosphere have occurred."
- IPCC (2021)

The question arises why the warming in the Arctic is so much stronger than elsewhere on the globe. Here *feedback mechanisms* come into play. These mechanisms can be self-damping (negative feedback) or self-strengthening (positive feedback) cycles. Global climate models are an essential tool to quantify these feedbacks. In the Arctic, several feedback mechanisms are causing the amplified warming. An overview of feedbacks in polar regions is given in Goosse et al. (2018). The radiative feedbacks are the Plank, lapse rate, surface-albedo, water vapour, and cloud feedback. Of these, the lapse-rate and surface-albedo feedback are currently considered the dominating feedbacks (Block et al., 2020; Pithan and Mauritsen, 2014). The total effect of the cloud feedbacks is one of the most uncertain feedbacks, and it is unclear whether it is positive or negative (Goosse et al., 2018). The adapted Figure 2 from Block et al. (2020) shows the global distribution of the contribution of the total cloud feedback to the multimodel-

Figure 1: "Arctic near-surface air temperature trends for the 49-year period 1971–2019 for the freeze-up season (October through May) and 'melt season' (June through September). The trend metric is the linear regression temporal slope multiplied by the time-span in years." This figure and caption are from AMAP (2021), free to use for educational purposes, and were published by the Arctic Monitoring and Assessment Programme (AMAP).

mean top of atmosphere (TOA) radiation feedbacks. They used simulations from the Coupled Model Intercomparison Project phase 5 (CMIP5). The cloud feedback shows different signs depending on the region and is marked as uncertain in almost every region. This uncertainty is largely connected to unresolved processes in global climate models (GCMs), including cloud microphysics, turbulence and convection, which cause a large spread in the cloud feedback between models (Ceppi et al., 2017). Besides the small-scale processes, large-scale processes such as poleward moisture and energy transport are occurring and as Jenkins and Dai (2022) formulated it, "[...] it is unclear what processes *cause* AA and what processes *result* from AA". Currently, there is the ambition to improve the process understanding by running global cloud-resolving (approx. <3 km resolution, see discussion in Satoh et al., 2019) simulations to avoid at least some of the parameterisation problems. For this, several unified modelling systems have been developed, including the ICON (ICOsahedral Non-hydrostatic) modelling framework, which enables climate, weather and large-eddy simulations with the same model (Crueger et al., 2018; Dipankar et al., 2015; Zängl et al., 2015). Being able to perform high-resolution simulations can further add great value when studying specific locations. This thesis uses cloud-resolving simulations and focuses on the Svalbard region.

One reason to focus on Svalbard is the strong warming occurring there. As previously mentioned, the warming of the Arctic is occur-

Figure 2: Global distribution of the contribution of cloud feedbacks to the multimodel-mean TOA radiation feedbacks (W m^{-2} K^{-1}). Positive feedback effects, causing an amplified warming, are indicated by positive values. Block et al. (2020) considered 13 CMIP5 models in this study, and hatched areas represent "areas where less than 12 models (92 % of data sample) agree with the sign of the multimodel-mean and are therefore considered to be insignificant". This figure is the subplot b from figure 2 published in Block et al. (2020) under the CC BY 4.0 licence.

ring at different speeds in different locations. In Figure 1, one can see that the region East of Svalbard shows the strongest warming between October and May compared to the rest of the Arctic. Already a decade ago, Førland, Benestad, et al. (2011) found an average winter temperature increase of 3.5 °C at single stations in Svalbard from 1981-2010 and a 0.5-1.0 °C increase in summer. Isaksen et al. (2022) reinforced these findings and discussed the impact of the pronounced warming of the Barents Sea. The strong warming of this area is believed to be partially connected to the sea ice decrease, the inflow of warmer Atlantic water and the advection of warm, moist air from the lower latitudes (Dahlke and Maturilli, 2017; Lind, Ingvaldsen, and Furevik, 2018). Therefore, there is great interest in the region concerning atmospheric research.

Svalbard provides one of the few locations in the Arctic where permanent observations can be made. In Ny-Ålesund, which is located in the west of Svalbard (78.9 °N, 11.9 °E; close-up map in Section 4.2 Figure 5), a research base was established and is operated year-round. Permanent measurement stations are scarce in the high Arctic. Thus, this location has been studied extensively and provides a multitude of different observational data sets (e.g. Ebell et al., 2020; Maturilli and Kayser, 2017; Nomokonova et al., 2019). The first study presented in this thesis (Chapter 5) makes use of some of this observational data to evaluate the performance of the atmospheric model ICON in the Arc-

tic. Due to the distinct features of the surrounding of Ny-Ålesund, glaciers, mountains, and fjords, current research also focuses on how representative this location is for the broader Arctic. A range of instruments enables the research of clouds and humidity and are partially used in this thesis. Why clouds are especially of interest is explained in the following section.

1.2 ARCTIC CLOUDS

Globally, clouds cover roughly 70 % of the Earth when looking from a satellite perspective (Stubenrauch et al., 2013). The Arctic is on the cloudier side, with spatial average values around 60-70 % during the winter and a maximum during the summer and early autumn with around 80-100 % cloud cover (Liu and Key, 2016; Mioche et al., 2015). These clouds play an essential role in the hydrologic cycle and impact the Earth's radiative budget. The physical processes relevant to clouds in the Arctic are the same around the globe. Nevertheless, certain types of clouds and connected dynamics are more common in the polar regions than in comparison to the mid-latitudes or tropics. Several factors contribute to this, possibly the most obvious being the absence of incoming solar radiation during the polar night. Another factor is that the surface is often covered by sea ice and snow, with high albedo. Further, the Arctic atmospheric boundary layer (ABL) is often stably stratified with frequent temperature inversions (Tjernström and Graversen, 2009), and humidity inversions (Solomon et al., 2011; Vihma et al., 2011). Maturilli and Kayser (2017) also found these frequent inversions, especially in winter, in Ny-Ålesund using an extensive set of radiosondes. Additional differences are the lower aerosol load in the Arctic (Chapter 3 in Lohmann, Lüönd, and Mahrt, 2016) and dryer atmosphere compared to lower latitudes. As a consequence of the lower specific humidity and less convection occurring in the Arctic, Arctic clouds are thinner and contain less water than mid-latitude clouds (Serreze and Barry, 2014). This entails polar clouds having a higher relative transmittance with consequences for the radiative budget. Due to the low temperatures in the Arctic, a substantial amount of Arctic clouds are mixed-phase, with Mioche et al. (2015) reporting an average occurrence of mixed-phase clouds (MPCs) around 30 to 50 % in the Arctic. For Svalbard, they report an even higher average percentage between 45 and 60 %. As this thesis focuses in parts on low-level clouds (LLCs), the next section will provide a more in-depth explanation of their occurrence, structure and dynamics.

OCCURRENCE AND COMPOSITION OF LLC More than half of the frequently occurring cloud types in the Arctic are low-level stratiform clouds (Eastman and Warren, 2010). Mioche et al. (2015) further

found that the occurrence of low-level MPCs, between 500 m and 3000 m, dominated the MPC occurrence in Svalbard. They found that during the winter months, more than 80 % of the MPCs were low-level. Mioche et al. (2015) used spaceborne remote sensing, which has higher uncertainties towards the ground. Gierens et al. (2020) and Nomokonova et al. (2019) in contrast, used ground-based remote sensing instruments located in Ny-Ålesund and confirmed the frequent occurrence of low-level MPCs. The amount of liquid-containing clouds follows a clear yearly cycle with a maximum in summer and fall and a minimum in winter, although the surface types play a role in this context. Clouds over the open ocean, for instance, have been found to have a higher LWP in comparison to those over permanent ice and land (Cesana et al., 2012; Yu, Taylor, and Cai, 2019). Another aspect of these liquid-containing clouds is that they have been found to be quite persistent. For many case studies, the persistency has enabled the analysis of the same cloud system for several hours to days (e.g. Shupe, Daniel, et al., 2008; Shupe, Kollias, et al., 2008; Solomon et al., 2011). Gierens et al. (2020) approached this statistically and found that persistent low-level MPC, with minimum 1 hr lifetime, covered 23 % of the analysed time. The persistence of Arctic LLCs can be better understood if one looks at the structure and dynamics in liquid-containing low-level clouds.

STRUCTURE AND DYNAMICS OF LIQUID CONTAINING CLOUDS

Arctic liquid-containing LLCs have been well researched, and much is known about their overall structure and the dynamics maintaining them. As described by Morrison, Boer, et al. (2012) and others, it has been observed that stratiform mixed-phase clouds have one or more thin supercooled liquid containing layers. These layers may also contain ice particles, which precipitate, creating a region of frozen hydrometeors below the liquid-containing layers. This causes a distinct structure with the liquid at the top of the cloud and frozen hydrometeors below. The supercooled liquid close to the cloud top further causes radiative cooling and, as a consequence, turbulence, which can also enhance the lifetime as the well-mixed cloud layer is maintained. Shupe, Kollias, et al. (2008) looked at low-level Arctic clouds and studied the impact of updrafts and downdrafts, which can act as sources and sinks for hydrometeors. They found that both the liquid water path (LWP) and the ice water path (IWP) increase when there are upward motions. Another factor which acts as a cloud water source is the entrainment in the upper cloud region, where an advected moisture influx can increase the cloud lifetime. Besides these in-cloud mechanisms, these clouds depend on the boundary layer structure. Previous studies have found that these clouds are often entirely or predominantly decoupled from the surface (Gierens et al., 2020; Solomon et al., 2011), which means that the surface mixed layers

Supercooled liquid: water in the liquid form below 0 °C.

LWP: Integrated liquid water in a column over a unit surface area.

IWP: Integrated ice water in a column over a unit surface area.

do not mix with the cloud-mixed layers. The lower tropospheric stability has also been found to control the LWP in Arctic clouds strongly. Murray-Watson and Gryspeerdt (2022) found that an increase in LWP is possible for high-stability conditions. They reason that stronger stability inhibits the mixing of moist and dry air, therefore maintaining the LWP. These studies show that Arctic low-level liquid-containing clouds depend on many factors, including meteorological features, which must be captured in models if one wants to simulate these clouds. Studies focused on process understanding in clouds benefit from our increasing ability to perform cloud and partially turbulence-resolving simulations. This enables a direct comparison with the existing long-term local measurements and campaigns.

1.3 CLOUD FEEDBACKS AND THEIR RELEVANCE FOR THE CLIMATE

THE CLOUD-RADIATIVE EFFECT To understand the relevance of clouds in the climate system, it is necessary to understand the role of clouds in Earth's radiative budget. As formulated by Ramanathan et al. (1989), the cloud radiative effect (CRE), also referred to as cloud radiative forcing, C is the sum of the shortwave (C_{SW}) and longwave (C_{LW}) clear-sky and all-sky radiative components.

$$C = C_{SW} + C_{LW} \tag{1}$$

$$\begin{aligned} &with \quad C_{SW} = S(\alpha_{clear} - \alpha) \\ &and \quad C_{LW} = F_{clear} - F \end{aligned}$$

where S is the solar irradiation (shortwave, SW) and α,α_{clear} are the albedo for all-sky and clear-sky conditions. F is the longwave (LW) radiation flux emitted into space for clear (F_{clear}) and all-sky (F) conditions. While the CRE can be calculated for the surface and the top of the atmosphere (TOA), the latter is generally used to quantify cloud feedbacks. Henderson et al. (2013) found that, on average, the net TOA CRE and the net surface CRE are negative, indicating that clouds overall cool the Earth. There are strong differences in the CRE at different locations depending on the incoming solar radiation, predominant cloud types, and surface types. Ramanathan et al. (1989) discusses that clouds generally have a higher albedo than ocean or land except when there is a snow or ice cover, which connects to the special circumstances of Arctic clouds mentioned previously. This means while in the mid-latitudes, a cloud may have a shortwave negative CRE (C_{SW}), emitting more SW radiation towards space than clear sky, this can be the opposite in the Arctic, depending on the surface type. Ebell et al. (2020) clearly show this difference for

different albedo types, where the net surface CRE is positive for high albedos and negative for low albedos. When looking at the Arctic, it is further obvious that there is no shortwave cloud forcing during polar night when there is no solar irradiation. This means that the CRE has a net warming effect at the surface during the polar night due to the downwelling LW radiation (Curry and Ebert, 1992; Henderson et al., 2013). Consequently, the CRE follows a clear annual cycle in the Arctic, where clouds warm the surface most of the year with a short cooling period during summer (Curry and Ebert, 1992; Shupe and Intrieri, 2004). Ebell et al. (2020) quantified the CRE for Ny-Ålesund and also found a positive net surface CRE during most of the year, except in summer. Their results gave a yearly average for the surface CRE of +11.1 W m^{-2}, indicating that clouds, on average, warm the surface in Ny-Ålesund. Another interesting aspect of the Arctic is that the combination of surface types, with clear and cloudy sky, creates a four-mode structure of the terrestrial net irradiance, where clear and cloudy and sea ice and ocean can be distinguished (Wendisch et al., 2019). From a climate perspective, changes in clouds that cause a change in the CRE are of interest as this will impact the Earth's energy budget. Cloud feedbacks describe how the clouds will react to the warming climate as part of the climate system to restore the Earth's radiative balance. Therefore, it is important to quantify the CRE and cloud feedbacks and to reduce the uncertainties related to clouds in climate models (Ceppi et al., 2017).

Several studies have looked into the cloud properties that influence the CRE in the Arctic. Shupe and Intrieri (2004) and Ebell et al. (2020), for instance, show that liquid-containing clouds have a much larger impact on the CRE than pure ice clouds. Ebell et al. (2020) show for Ny-Ålesund that the LW surface CRE increases with increasing LWP until it converges around 75 W m^{-2} for dense clouds. A study by Bennartz et al. (2013) showed that low-level liquid clouds contributed to the melting of the Greenland ice sheet during the period which they studied. They found that thin low-level liquid clouds with a LWP between 10 and 40 g m^{-2} can cause more substantial warming than liquid-containing clouds with higher LWP. The thin liquid clouds lie in an optical thickness range that causes downward solar radiation to penetrate the cloud but inhibits the outward longwave radiation from escaping, therefore causing more substantial warming of the surface layers. Representing thin and supercooled liquid-containing clouds is challenging for climate models as they must parameterise the microphysical processes and aerosols. Even in high-resolution simulations, such cloud microphysical parameterisations must be used. Although cloud-resolving simulations at least avoid the issue of convection parameterisations, these microphysical parameterisations still present considerable challenges (Morrison, Lier-Walqui, et al., 2020). Addi-

tionally, accurate and polar covering observations of LWP are still lacking (Kay et al., 2016). Such deficiencies are an issue because estimating how much Earth's climate will change requires an accurate representation of the energy budget. If one cannot accurately model clouds, one cannot accurately predict changes in the CRE and, consequently, how cloud feedbacks may impact the Arctic amplification. A study by Zelinka et al. (2020) looked into differences between the *effective climate sensitivity* (ECS) of CMIP5 and CMIP6 models and found an increase in the ECS in the newer model versions. They attribute this mainly to strengthened cloud feedbacks and point out that there are still several open questions relating to clouds in models. Other studies focusing on the Arctic have shown that it is unclear whether cloud feedbacks are in total negative or positive due to the different impacts they can have on the radiative budget (Block et al., 2020; Pithan and Mauritsen, 2014). One can see that it is necessary to understand the role of clouds in the Earth's energy budget to understand why research in this field is necessary. In many parts, this thesis looks at clouds; the recurring theme is the phase-partitioning of clouds. To further provide some background on the explicit interest in the phase-partitioning of clouds, the following section gives an overview of the cloud-phase feedback.

Effective climate sensitivity: "[...] global surface temperature that would restore TOA energy balance in response to an instantaneous doubling of CO_2." (Zelinka et al., 2020)

THE CLOUD-PHASE FEEDBACK The cloud-phase feedback, as described by Mitchell, Senior, and Ingram (1989), is very challenging to quantify due to the difficulties and differences in how the liquid and ice phases are parameterised in general circulation models (GCMs). The feedback is based on the fact that the liquid part of clouds will increase in a warmer atmosphere. Liquid clouds are optically thicker than ice clouds as they contain more hydrometeors and scatter sunlight more efficiently. Further, they can live longer than ice clouds, which have particles with higher fall velocities, causing a higher precipitation rate. Therefore, it is reasoned that if the liquid phase increases in clouds, this will decrease the warming and act as negative feedback (Storelvmo, Tan, and Korolev, 2015). The work by Komurcu et al. (2014) showed how six GCMs, which they compared to satellite data, had very different LWP and IWP values both between the models and in comparison to the satellite data. They also found large differences between the models in the supercooled liquid fraction of over 70 %. Cesana et al. (2012) did a similar experiment and found that their chosen climate model could not reproduce the liquid water amount in Arctic clouds compared to satellite data, which caused an incorrect net surface radiative flux. Ceppi et al. (2017) discusses that the spread between modelled high-latitude cloud phase changes, which contribute to a change in the optical cloud depth, are mainly caused by different microphysical parameterisations. These examples show how hard it is to estimate the impact of the cloud-phase feed-

back when the models have such large discrepancies and that improvements in the phase partitioning are necessary.

INTERACTIONS BETWEEN AEROSOLS AND CLOUDS This thesis focuses on cloud properties in models, and therefore, aerosols also play a role. Aerosols can act as cloud condensation nuclei (CCN) and ice nucleating particles (INPs), enhancing the formation of droplets and ice particles (more in Section 3.3). In large-scale models, such as ICON, these aerosols are parameterised using CCN activation and INP nucleation schemes. Generally, two main indirect aerosol effects on clouds are discussed in the literature. The first one is the Twomey effect (Twomey, 1974, 1977), which describes the impact of aerosol changes on the optical properties of a cloud. If more aerosols are available and at constant LWP, cloud droplets will decrease in size while the droplet number concentration increases, causing an increase in optical thickness. This will increase the cloud albedo and, therefore, change the CRE, which is believed to enhance the cooling effect of clouds on the global average. The fundamental theory behind the Twomey effect has been well established, but it remains difficult to quantify the exact impact on the CRE. Quaas et al. (2020) mention several issues making it hard to quantify the Twomey effect, as large-scale observations of small-scale processes are currently not possible to the extent necessary. The second indirect aerosol effect is the Albrecht effect as described by Albrecht (1989). The theory is that an increase in CCN can increase cloud lifetime by suppressing precipitation formation. Increasing the number of CCN affects the droplet size distribution, causing changes in the liquid water content of the clouds. How exactly these connections between CCN and cloud properties work is still not fully clear though (Khain and Pinsky, 2018). Mauritsen et al. (2011) looked at both indirect aerosol effects for Arctic clouds and the radiative forcing connected to these. They found that the cloud formation was limited by CCN availability and that small changes in CCN concentrations could have large impacts on the CRE in these low CCN regimes. Further, they discuss the competition of cooling and warming aerosol indirect effects, where seasonality plays a role, and argue that the aerosol indirect effect likely causes warming from the average climatological perspective. INPs, which have much lower concentrations than CCN (Lohmann, Lüönd, and Mahrt, 2016; Morrison, Boer, et al., 2012), come into play in cold clouds. A recent review by Burrows et al. (2022) highlighted that for INPs, there are still large challenges in bridging the gap between observations and models. On both sides, improvements are necessary to understand and quantify the impact of aerosols as INPs on clouds. In light of climate change, there are many Arctic-specific questions related to how the INP and CCN sources, concentrations and compositions will change in the future (Schmale, Zieger, and Ekman, 2021).

For instance, the impact of the retreating sea ice, changes in precipitation type, and changes in natural aerosol sources are being discussed. This paragraph just mentioned some of the main aerosol-cloud interactions and considerations related to INPs and CCNs in the Arctic. It does not cover all processes, as that would go beyond the scope necessary in this thesis. As one can tell, though, aerosol-cloud interactions have long been a topic. While many theoretical concepts have been established in the past, the challenge nowadays is to quantify these processes and their (future) impacts. Capturing these interactions is another challenge in atmospheric models. Although it is possible to expand models to include more sophisticated aerosol emissions, transportation, chemistry and dynamics, which is done, for instance, in ICON-ART (ICOsahedral Nonhydrostatic model with Aerosols and Reactive Trace gases, Schröter et al., 2018), this can cause a considerable computational slowdown. Additionally, one cannot fully constrain such simulations as observations are often unavailable. Therefore, it is necessary to understand how the current nucleation and activation parameterisations in models, which do not include a chemical transport model, influence simulated clouds.

SUMMARY OF MAIN POINTS Several different topics have been addressed in the motivation of this thesis, explaining why this research was conducted and how it fits into the larger scientific picture. These are the major points to take away:

- The Arctic is undergoing rapid changes, and to understand and predict them, the region must be studied.
- Large uncertainties in climate projections can be attributed to the inaccurate representation of cloud microphysical processes in parameterisations as cloud properties impact the Earth's radiative budget.
- The phase-partitioning of mixed-phase clouds is often not correctly represented in atmospheric models.
- Cloud aerosol interactions are yet to be fully understood and currently cannot be accurately constrained in models, especially in the Arctic.

As discussed, there are different ways to address these challenges. In this thesis cloud-resolving simulations are used in combination with observations to improve our understanding of how aerosols and cloud microphysical processes impact the phase-partitioning in Arctic clouds.

2 SCOPE OF THIS THESIS

2.1 OBJECTIVES

This thesis focuses on three main research questions, each with a dedicated chapter in the results section. The studies build on each other, and in the following section, the research questions with a summary of the related study and its context are given.

> First research question: How well does ICON-LEM perform in a complex Arctic environment with respect to humidity and clouds?

The first question, addressed in Chapter 5, sets the focus on the Arctic. As discussed in the introduction, this region is of high interest due to the rapid changes in its climate system. This study provides a baseline for the performance of the state-of-the-art operational model ICON in an environment for which it was originally not specifically developed. Further, the focus on clouds and humidity connects to the larger issue that models still struggle with uncertainties in this respect. For this purpose, the data from several months of daily semi-operational simulations was used to evaluate the performance of the model setup in an Arctic environment. This research was done using various observations as reference, and overall one could see that ICON-LEM performs quite well in many aspects (e.g. temperature and wind profiles and integrated water vapour). Some limitations were found regarding the liquid water path and precipitation. Another shortcoming of the model was the substantial underestimation of liquid-containing clouds. This study is valuable for all those who want to use ICON, which was originally tuned for the mid-latitudes in the Arctic. The study also provides a benchmark which shows where improvements are necessary for the ICON model in an Arctic setup.

> Second research question: How does a change in the INP and CCN parameterizations impact the liquid water path and supercooled liquid fraction?

As pointed out in the first study, the used ICON setup struggled with the liquid water in clouds. Therefore, the second study (Chap-

ter 6) explores how a change of aerosols impacts the liquid water in clouds. To achieve this, two months of simulations with two different aerosol schemes are compared. The first setup uses the default settings, which are based on European aerosols, while the second setup is more oriented towards maritime clouds, which are more similar to Arctic clouds. These results showed that the liquid water path distribution was more fitting for the Arctic. It did not increase the amount of clouds containing liquid, though. Therefore, this still remained an open issue. Additionally, observational data was used to quantify whether improvements in the LWP could be seen in the simulations with the maritime aerosols. Such improvements could be seen for the distribution of lower LWP values, which occur most frequently, and therefore this setup was kept for the last study.

Third research question: Which microphysical processes dominate the phase-partitioning in low-level Arctic clouds?

The last study (Chapter 7) is focused on the microphysical processes in low-level Arctic clouds. The goal is to improve our understanding of microphysical processes in Arctic clouds, as this is necessary if one wants to represent them better in climate models. Connecting to the previous two studies, this study addresses the underlying problem that representing supercooled liquid remains a difficulty in ICON-LEM. While aerosols drastically impact the amount of liquid water in clouds, the previous study showed that microphysical processes must also be improved to sustain liquid water in clouds. Therefore, this study looks into microphysical processes which change the phase-partitioning of a cloud. Here, the low-level clouds are the main focus as these often are mixed-phase. To obtain the process rates from previous simulations, a diagnostic tool (microphysical wrapper) was developed and implemented and enabled the analysis of eight months of daily simulations. The results give an idea of which processes could potentially be modified to reduce the lack of liquid water. Additionally, an overview is given of the regimes in which a process is active. These insights can help to set the focus for future model improvements and the diagnostic tool can be used to fill gaps in our understanding of cloud microphysics.

Each of these studies was only possible due to two major methodological achievements. The first achievement is the setup of continuous cloud-resolving simulations for an Arctic environment that provide daily insights. A collection of simulations has been created, which covers ca. 3 years. This setup is described in the method Section 4.2. Another achievement was the implementation of a "microphysics wrapper", which enables the output of microphysical process rates for

a two-moment microphysical scheme used in the ICON model. An overview of the capabilities and implementation are given in Section 4.3.

2.2 ETHICAL CONSIDERATIONS OF THIS RESEARCH AS A GUEST IN THE ARCTIC

The Arctic is home to approximately 4 million people, of which many belong to various different Indigenous Peoples, for whom it is difficult to give an accurate estimate (Larsen and Fondahl, 2014). These people are already directly impacted by the changing environment. Wildfires, pollution, sea ice melting, extreme events and permafrost thawing are some of the major threats to their traditions and livelihoods. An example given in the report by AMAP (2021) is that hunters in northwest Greenland report a decrease in the period when travel by dogsled on sea ice is possible, from 5 to 3 months. In addition to the people living in the Arctic there are many parties with different, in parts conflicting, interests in this area. This work, for instance, is funded by the Deutsche Forschungsgemeinschaft (German Research Foundation, TRR 172), making it clear that in a country far from the Arctic, such as Germany, there is also an interest in the Arctic region. It must further be noted that the funding of this project is solely for German institutes and raises the question of how we can avoid doing "helicopter research" [1]. A lot of knowledge already exists in Arctic communities and we must critically evaluate how we do our science and how we can avoid being part of a neo-colonialist scientific culture. I, too, am a guest in the Arctic and not exempt from the critique. I have several times in my scientific surroundings experienced a disregard towards the Arctic wildlife, Indigenous Peoples and local communities. Efforts, for example, from publishers (Nature, 2022), or in the collection of data (e.g. Hauser et al., 2023) are already being undertaken to improve the way we practice science, but the scientific community still has a long way to go. The creation of knowledge and understanding continues and this thesis is just a very small piece in an enormous puzzle. Finding and putting the puzzle pieces together is a communal task and must include those living in the regions we study and I sincerely hope putting the pieces together will convince and enable us to better protect the wildlife and livelihoods many humans are currently destroying.

1 "'Helicopter research' occurs when researchers from high-income settings, or who are otherwise privileged, conduct studies in lower-income settings or with groups who are historically marginalized, with little or no involvement from those communities or local researchers in the conceptualization, design, conduct or publication of the research." (Nature, 2022)

Part II

THEORY & METHODS

3 CLOUDS IN ATMOSPHERIC MODELS

3.1 THE ICON MODELLING FRAMEWORK

Before one begins to simulate a cloud, one must have an atmospheric model, which is, in our case, the ICOsahedral Non-hydrostatic modelling framework ICON Crueger et al., 2018; Giorgetta et al., 2018. That ICON is a modelling framework means that different resolutions, covering several scales, can be run using the same model. For instance, it is possible to run it as a global climate model (GCM), for numerical weather prediction (ICON-NWP; Zängl et al., 2015) and as a large-eddy model (ICON-LEM; Dipankar et al., 2015; Heinze et al., 2017). In all versions, the underlying physics is described by the governing equations for the conservation of mass, energy, momentum, and the ideal gas law, but different assumptions must be made depending on the version. In this thesis, two ICON versions are used, ICON-NWP and ICON-LEM. Using this approach enables the same subgrid-scale parameterisations where possible and the same underlying implementation of the dynamical part. The parameterisations represent processes which cannot be resolved given a certain grid size. This work uses the ICON-NWP version to force the ICON-LEM simulations. This means the boundary and initial conditions for the ICON-LEM simulations stem from the ICON-NWP simulations, as the simulations are run on limited areas. The simulations that were primarily evaluated were run with ICON-LEM. To explain why mainly the LEM version of ICON was used, the following short rhyme taken from Richardson and Lynch (2007) provides a starting point

> "Big whirls have little whirls
> which feed on their velocity
> and little whirls have lesser whirls,
> and so on to viscosity."
> - *Lewis Fry Richardson.*

Richardson was referring to the energy cascade of eddies with different sizes. As an NWP cannot resolve these eddies, which have a characteristic length from approximately 2 mm to 2 km, one can use Large-Eddy Models (LEM) with mesh sizes of O(10 m). How much of the energy spectrum can be resolved is determined by the mesh size in combination with the integral length scale (averaged eddy size) and sets the limit below which turbulence must be parameterised. Further, one must keep in mind that the eddy size, which can be resolved, is always larger than the actual mesh size.

Non-hydrostatic: Allowing vertical motions

To explain the concept behind turbulence parameterisation choices in more detail, it is worth taking a step back to look at traditional mesoscale NWP simulations, e.g. the ones used as forcing in this thesis. There, the non-hydrostatic governing equations for a rotating sphere are solved (see Gassmann and Herzog, 2008; Prill et al., 2020). These equations are the continuity equation for the conservation of mass, the first law of thermodynamics giving conservation of energy, the Navier-Stokes equation giving the conservation of momentum, the equation of state of an ideal gas, and additionally the equation of conservation of water. As mentioned above, the NWP cannot resolve turbulence; therefore, in ICON-NWP Hesselberg averaging is used to decompose each field ϕ into the density-weighted mean $\widehat{\phi}$ and its deviation ϕ'' (Hesselberg, 1926):

$$\phi = \widehat{\phi} + \phi'' \ . \tag{2}$$

This approach is similar to using the more commonly known Reynolds average ($\overline{\phi}$), except that it includes the density weighting ($\widehat{\phi} = \overline{\rho\phi}/\overline{\rho}$). For this reason, one may also speak of a RANS model indicating that one uses the Reynolds-averaged Navier-Stokes equations. From a model perspective, the decomposition means that there is a resolved component of the variable ϕ in the form of $\widehat{\phi}$ as well as an unresolved (subgrid scale) component ϕ''. This subgrid scale component represents the turbulent diffusion that must be parameterised in the NWP model. In ICON-NWP, there are two turbulence schemes which are used by default, one for the free troposphere (TURBDIFF, Raschendorfer, 2001) and one for the surface layer (TURBTRAN, Prill et al., 2020; Raschendorfer, 2001). If one now decreases the horizontal resolution and begins to resolve some of the large eddies, the deviation ϕ'' from the mean state becomes partially resolved. This is where Large-Eddy models (LEMs) or simulations (LES) come into play.

Now, the tricky question is how much of the turbulence can be resolved in a LEM. The underlying idea of how to approach this problem is to use low-pass filtering applied to the Navier-Stokes equations. The low-pass filter uses a cutoff frequency (a length and time scale), below which the small-scale turbulence is discarded. As formulated by Davidson (2004) "The idea of LES is to compute both the mean flow and the large, energy-containing eddies exactly". This is often advantageous as the large scales mostly dominate important processes such as mass transport. As described in Dipankar et al. (2015), ICON-LEM uses a low-pass filter to filter the turbulent fields as:

$$\phi = \tilde{\phi} + \phi' \ , \tag{3}$$

where $\tilde{\phi}$ is Favre-filtered. This is not the same approach as using the Hesselberg average in Equation 2, which was mentioned above. While both $\tilde{\phi}$ and $\widehat{\phi}$ represent the resolved part, $\widehat{\phi}$ represents just

the mean flow while $\tilde{\phi}$ represents the mean state and the large-scale eddies. The difference is that in the LEM Equation 3, one assumes one can resolve the large-scale eddies, included in $\tilde{\phi}$ so that only the small-scale ones must be parameterised (ϕ'). In the NWP, the large eddies must be completely parameterised (ϕ'' in Equation 2). In ICON-LEM, the subgrid-scale turbulence is parameterised using a 3D-Smagorinsky scheme, with adaptations following Lilly (1962) (Dipankar et al., 2015).

It is necessary to mention that model resolutions can lie between the traditional mesoscale NWP (RANS) and LEM resolutions. Such simulations are considered to be in the turbulent "grey zone", and Honnert et al. (2020) estimates that simulations with mesh sizes between 200 m and 2 km fall into this category. Currently, this grey zone is an active area of research as the increasing computational resources have made hectometer simulations more attractive. In this grey zone, one is confronted with the issue that neither the assumptions regarding turbulence parameterisations made in NWP nor in LES hold (Honnert et al., 2020). There is a movement towards creating grey zone or scale-aware turbulence parameterizations, although none of these are available at this point in ICON.

Besides the subgrid-scale motion, which also includes the turbulent diffusion of moisture, other cloud properties must be parameterised to a certain extent. In ICON-NWP, the cell size is mostly too large to represent single clouds. Therefore, a cloud-cover parameterisation is used to estimate how much of the cell is covered by clouds. The diagnostic scheme, implemented in ICON, combines the information from the turbulence, convection and microphysics parameterisations to derive the cloud distribution (Köhler, 2020). For cloud-resolving simulations, an all-or-nothing scheme (Sommeria and Deardorff, 1977) is used, where each grid cell is either cloudy or clear. As discussed in Satoh et al. (2019), "No consensus has emerged as to the resolution at which a model can be considered cloud-resolving". They further point out though that currently, resolutions around and below 4-3 km are considered "cloud-resolving". They mention that generally, resolutions around 1 km and finer are considered to resolve convection enough to enable statistical studies of a cloud/cloud system. Therefore, convection parameterisations used in NWP models can be turned off at the latest at subkilometer resolutions. In ICON, there is further the option to only use a shallow convection parameterisation for cell sizes below 5 km. As cloud properties are defined by processes on multiple scales, including the microscale, the microphysical properties of a cloud are separately parameterised. The concept of microphysical parameterisations as well as details on the parameterisation chosen in the ICON simulations performed for this work, are

given later.

Another reason one uses hectometer simulations is that the higher the resolution, the better the topography and surface types can be resolved. This is especially valuable in the Svalbard Archipelago as it is a complex environment with mountains, glaciers, fjords, open oceans, and decreasing sea ice. Fig. 1 in Dekhtyareva et al. (2018) demonstrates what happens when one uses a low-resolution model. The figure shows that in ERA-Interim, the "Ny-Ålesund cell" is centred ca. 19 km to the south of Ny-Ålesund on a glacier-covered mountain. This is obviously a disadvantage in an environment with heterogeneous surface types and pronounced orography. For the Arctic, the availability of highly resolved orography is more limited in ICON in comparison to the mid-latitudes. Currently, two different choices can be made for the orography in the Arctic, which are the GLOBE (1 km resolution; Hastings et al., 1999) and the recently added MERIT-DEM (90 m resolution; Yamazaki et al., 2017) data sets (Asensio et al., 2021).

Regular icosahedron

Now that the advantage of using different resolutions has been discussed, it is worth taking a moment to understand what "resolution" means in ICON. The "icosahedral" in the name ICON already hints towards a speciality of the grid. ICON uses a staggered C-grid, which is based on a regular, convex icosahedron which has 20 equilateral faces that are shaped as triangles (Wan et al., 2013; Zängl et al., 2015). These faces are refined systematically to create the grids with the desired resolution. These grids are termed as "RnBk"-grids, where n and k determine the degree of refinement and give the number of cells as $n_{cells} := 20n^2 4^k$ (details in Zängl et al., 2015). The term "resolution" can describe several features of a triangular cell, and in this work, generally, the edge length of a cell is meant. In other modelling contexts, the resolution can be given as the edge length of a square. This length is shorter than that of a triangle edge with the same area as the square. One can easily approximate the corresponding square edge length using the triangular edge length $\overline{\Delta x}$ as $\frac{2}{3}\,\overline{\Delta x}$. For any chosen resolution in ICON, one must parameterise the microphysical processes. As the results in this thesis include an analysis of these microphysical processes, the subsequent section will give an introduction to essential concepts in this regard.

3.2 MICROPHYSICAL MODELS

There are quite a few books in which cloud microphysical processes and their parameterisations are explained. Two of these are used in the following sections as general references: Khain and Pinsky (2018) and Lohmann, Lüönd, and Mahrt (2016). Further, in this work, the term "cloud microphysical parameterisation" is sometimes shortened

to "microphysical parameterisation" or "microphysical scheme".

The question of how to simulate a cloud and what to parameterise is addressed by various different approaches as there is one fundamental limiting aspect: the length and size scales. Depending on what one wants to achieve, i.e. a climate projection, a weather forecast, or the collision of two droplets in a cloud, the answer to this question will be different (Morrison, Lier-Walqui, et al., 2020, Figure 2). In this work, processes below the meso-γ (<2 km) are of interest, and the main grid resolution used in this thesis lies at around 600 m. Therefore, microphysical processes cannot be resolved and must be parameterised, while it is assumed that the convection parameterisation can be turned off, as discussed above. Several methods exist to parameterise the cloud microphysical processes, and a short overview is given here. More background will be provided regarding bulk schemes as this thesis focuses on a two-moment bulk scheme. The underlying problem which must be solved is the evolution of a hydrometeor population with time. Following Morrison, Lier-Walqui, et al. (2020), the most general form of this evolution can be written as

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f - \frac{1}{\rho}\frac{\partial(\rho V f)}{\partial z} = \left(\frac{\partial f}{\partial t}\right)_{\text{diff}} + P_1 + P_2 + ...P_N \ . \tag{4}$$

There, f describes the hydrometeor population distribution, $\mathbf{u}$ is the wind vector, ρ the air density, V the particle fallspeed, and P_1, P_2, ... P_N are single microphysical processes (i.e. riming, condensation, etc.). $\left(\frac{\partial f}{\partial t}\right)_{\text{diff}}$ describes the diffusion in physical space. Later on, the specific definition of f in bulk models will be discussed.

DNS AND SUPER-PARTICLES The smallest possible simulation of cloud microphysics is a particle-by-particle direct numerical simulation (DNS). These simulations must have very fine resolutions (< 1 mm) but have the advantage that they can resolve most of the turbulent flow. Hydrometeors can be simulated in these simulations as point particles using Lagrangian dynamics (Golshan et al., 2021). Another method is the use of a Monte-Carlo model to simulate the evolution of so-called "super-particles" (e.g. Brdar and Seifert, 2018; Shima et al., 2009). This approach enables an in-depth study of cloud processes, but the simulation domains for DNS are strongly restricted by the high computational resources needed to perform such simulations.

MACHINE LEARNING APPROACHES The most recent method used to understand and improve microphysical parameterisations is machine learning (ML) methods. While some research groups aim to replace physical parameterisations completely, others advocate to use

ML to tune the parameters of the physical parameterisations. One example of the latter is a tool introduced by Couvreux et al. (2020), which enables the "learning" of suitable parameter choices for a given parameterisation. A study by Seifert and Rasp (2020) aimed at predicting warm-rain process rates solely using neural networks, which each represent one process. A similar approach was used by Gettelman et al. (2021) although in contrast to Seifert and Rasp (2020), Gettelman et al. (2021) used a bin scheme as a model to learn from and not a super-particle model. These methods have the advantage that ML algorithms can learn from highly resolved simulations and run on larger scales with much lower computational times. The downside is, though, that they can behave nonphysically, do not necessarily improve our understanding of microphysical processes, and can behave unexpectedly in regimes on which they have not been trained (e.g. climate change scenarios).

SPECTRAL BIN MODELS Spectral bin models offer the ability to directly represent the mass distribution of different hydrometeor types without making preset assumptions of the particle size distribution (PSD). In this approach, Equation 4 is computed for several mass bins, which has the advantage that fewer assumptions are made and a more extensive range of cloud conditions can be represented. A disadvantage is that the higher computational cost compared to bulk models makes it less favourable for large-scale simulations.

MICROPHYSICAL BULK MODELS Microphysical bulk models are the most commonly used schemes in current GCMs and cloud-resolving models as they are fast and can cover different levels of complexity. In bulk models, the computation of process rates that change either the number concentrations and/or mass of a hydrometeor is based on analytical equations.

When it is not possible to represent single hydrometeors, one can instead compute the characteristics of the hydrometeors for an entire volume. The PSD is expressed as a function of the particle mass m to achieve this, $f(m)$. Computing the moments of the PSD gives physical insights into a cloud volume. A moment of order k for $f(m)$ is defined as:

$$M^k = \int_{m_{min}}^{m_{max}} m^k f_m(m) dm \tag{5}$$

This gives the *particle number concentration* N as the zero-order moment.

$$M^0 = N = \int_{m_{min}}^{m_{max}} f_m(m) dm \tag{6}$$

And as first-order moment the *mass densities* L.

$$M^1 = L = \int_{m_{min}}^{m_{max}} m f_m(m) dm \tag{7}$$

This explains the naming of one-moment schemes, which mostly predict the particle mass density L and two-moment schemes, which in addition to L, also predict the number concentration N. In accordance with Equation 4, the bulk scheme predicts the change of each moment M^k, which replaces f in the mentioned function.

In this thesis, the focus lies on the Seifert and Beheng (2006) scheme (SB06), which is a two-moment scheme that predicts both N and L, although L is converted into the mass-mixing ratio in the output of ICON. The PSD ($f(m)$), can be approximated by a generalized Γ-distribution (Chapter 2, Khain and Pinsky, 2018; Seifert and Beheng, 2006, for more details). Another important concept is that hydrometeors can have very different properties (density, size, terminal fall velocity, etc.). Therefore, it is not feasible to describe all hydrometeor types using a single PSD. The approach chosen in SB06 was to define five hydrometeor types: cloud droplets, raindrops, cloud ice, snow, and graupel. Later, an additional hail type was added (Blahak, 2008). Accordingly, in the ICON two-moment scheme, six hydrometeor number concentrations and mass mixing ratios are computed. An example of an alternative way to treat the hydrometeor types is the predicted particle properties (P3) scheme by Morrison and Milbrandt (2015).

There they use a single ice category but use four prognostic mixing ratio variables (total ice mass, ice number, the ice mass from rime growth, and the bulk rime volume) to describe different ice particle regimes. There are many different processes that impact the number concentration and mass density of each hydrometeor type. In the last study presented in this thesis, these processes are evaluated for low-level Arctic clouds. Therefore, the following section will provide an overview of cloud microphysical processes with reference to their implementation in SB06 in ICON (more details in Khain and Pinsky, 2018; Lohmann, Lüönd, and Mahrt, 2016).

3.3 MICROPHYSICAL PROCESSES

3.3.1 *Saturation, nucleation and activation*

Two important variables in cloud microphysics are the saturation vapour pressure e_s and the saturation S. e_s is defined as the water vapour pressure e, which is in equilibrium with a liquid or solid water surface, i.e. the air is saturated. The dependency of e_s on the temperature is described by the well-known Clausius-Clapeyron equation.

This is also true below 273.15 K, where water can be liquid and solid. In this regime, two different saturation vapour pressures, one for liquid $e_{s,w}$ and one for solid water $e_{s,i}$, exist. The ratio of the vapour pressure e and the saturation vapour pressure can be used to calculate the saturation $S = e/e_s$ of an air parcel, with respect to liquid ($S_w = e/e_{s,w}$) or ice ($S_i = e/e_{s,i}$). Due to the molecular structure of ice, the saturation vapour pressure is lower with respect to ice than with respect to liquid at the same temperature (below 273.15 K). An air parcel is unsaturated if $S < 1$, saturated if $S = 1$, and supersaturated if $S > 1$. In models, empirically derived equations are used to describe the saturation vapour pressure e_s.

Droplets and ice particles can form in cases where $S > 1$. Generally, a cloud condensation nuclei (CCN) is required for a cloud droplet to form. The CCN must reach a certain size ("critical radius") to achieve droplet formation, which it can only do in supersaturated air. This critical radius depends on the aerosol properties, which can vary depending on the CCN. Above this radius and given that $S > 1$, the droplet can grow as long as vapour is available to condensate on the CCN; one calls this an "activated CCN". In a model, one describes this droplet formation using a *CCN activation* scheme which may or may not include different types of aerosols.

The formation of ice can occur homogeneously or heterogeneously and is termed as *nucleation* or *freezing*. Generally, supercooled liquid droplets spontaneously freeze below 0 °C with increasing likelihood for colder temperatures until they are all frozen around -38 °C. Homogeneous freezing of droplets in the atmosphere is unlikely as no INP is involved in this process. In SB06, this process is implemented for temperatures below -30 °C, and below -50 °C all droplets are instantaneously frozen. Homogeneous freezing may also refer to the freezing of a liquid solution, and in SB06, it is treated in the homogeneous and heterogeneous nucleation routine. Deposition nucleation, immersion freezing and contact freezing all require an ice nucleus and are different forms of *heterogeneous nucleation*. As the name indicates, deposition nucleation describes the deposition of water vapour molecules onto an INP (also ice nuclei IN). Lohmann, Lüönd, and Mahrt (2016) and Burrows et al. (2022) mention, though, that it is currently debated whether deposition nucleation does occur at all. Immersion and contact freezing both involve cloud droplets which are frozen either because they already contain an ice nucleus (immersion freezing) or because they come into contact with one (contact freezing). Different aerosol types can act as CCNs and INPs, and while further aspects related to CCNs and INPs are discussed in Chapter 6, details on this go beyond this thesis. Different ways to parameterise the INP nucleation and CCN activation are possible, and Chapter 6 will introduce

those which are used in this thesis in greater depth. The basic idea behind these parameterisations is to create functions that "activate" the aerosols, increasing the number and mass of droplets or ice based on thermodynamic model variables such as saturation or vertical wind. Generally, these parameterisations are based on observational data, laboratory experiments, aerosol models and high-resolution simulations to derive, verify and tune these functions. The challenge of these schemes is that one must combine the complexity of aerosol-cloud interactions with the need to simplify in a model. A difficulty faced in regard to heterogeneous nucleation/activation parameterisations is the large variability and uncertainties related to CCN and INP (Burrows et al., 2022; Schmale, Zieger, and Ekman, 2021).

3.3.2 *Processes in liquid or ice clouds*

VAPOUR PHASE PROCESSES After the creation of a droplet or an ice particle, the hydrometeor can grow through water vapour diffusion onto the hydrometeor if the air surrounding the particle is supersaturated. This is termed condensation for liquid and deposition for ice particles. The availability of water vapour limits the growth by diffusion, and in unsaturated air, evaporation or sublimation will set in and act as a sink to the liquid or frozen mass, respectively. Precipitation is another sink of moisture, but for a hydrometeor to reach the size at which it will precipitate, further growth processes must set in. The ICON model aims to maintain an equilibrium between water in the different phases. To achieve this, a saturation adjustment is used to either condense or evaporate onto/from water droplets in saturated or unsaturated grid boxes. Rain evaporation is treated separately as part of the microphysics scheme, not the saturation adjustment. This saturation adjustment is not part of the microphysical scheme but is implemented separately. The growth and decrease of frozen particles by deposition and sublimation are implemented as part of the microphysical scheme.

LIQUID COLLISIONS Liquid particles can grow further by colliding and coalescing with other liquid particles, termed as *collision-coalescence*. The collisions can cause drop breakup, which limits the liquid particle growth. In the ICON two-moment SB06 scheme, a differentiation is made between the collision of cloud droplets (c) and raindrops (r). There exits self-collection ($c + c \rightarrow c,\ r + r \rightarrow r$), autoconversion ($c + c \rightarrow r$), accretion ($r + c \rightarrow r$), and breakup ($r + r \rightarrow r$). Only by growing via mechanisms that do not involve the vapour phase can a large raindrop develop out of a cloud droplet. Consequently, these processes are important for the creation of warm rain.

FROZEN COLLISIONS Same as for liquid particles, frozen particles may collide with each other due to different terminal velocities or turbulence. This process is termed aggregation, and in SB06 in ICON, this is implemented for all frozen hydrometeors. How likely it is that two particles will stick together depends on their sticking efficiency. Frozen collisions can further act as secondary ice production mechanisms. Secondary ice production is understood as the process of ice multiplication, which does not form through aerosol-mediated nucleation. This ice multiplication is relevant as it has been found that the number of ice particles can be much larger than the number of INPs. In cases where frozen particles collide, the particles can fracture, causing the production of small ice fragments, which can act as new INPs. A study by Sotiropoulou et al. (2020) found that implementing break-up due to ice-ice collisions was crucial to get the ice number concentrations into a more realistic range. As secondary ice production mechanisms are still relatively unclear, they have only partially been included in large-scale models.

SEDIMENTATION To model surface precipitation, it is necessary for sedimentation to be parameterised, and it is called after the microphysics in SB06 in ICON. Generally speaking, hydrometeors of different sizes, shapes and densities have different fall velocities. To deal with these differences, the mean fall velocity of each hydrometeor type is computed separately. As cloud droplets are assumed to have a neglectable mean fall velocity, no sedimentation is computed for them.

3.3.3 *Processes in mixed-phase clouds*

Mixed-phase clouds add another level of complexity to the discussion. As discussed in Korolev et al. (2017), further research in all directions, laboratory, remote sensing, in-situ, theory, and modelling, is still required to fully understand the mechanisms and accurately describe the microphysical processes in MPCs. In the previous paragraphs, the processes which occur in pure ice or liquid clouds were described. Therefore, they are not repeated, and only interactions between liquid and ice hydrometeors are introduced.

RIMING In areas where liquid and frozen hydrometeors are present, riming can occur. This is the case when liquid and frozen hydrometeors collide, causing the liquid to freeze and the frozen particle to grow. In SB06 in ICON, riming includes the Hallet-Mossop secondary ice production (rime splintering, Hallett and Mossop, 1974). Therefore, the ice number concentration can increase due to rime splintering. It also includes enhanced melting if the temperature is above 0 °C, which causes the decrease of the rimed particle mass and the increase

of rain mass. Additionally, ice and snow may be converted to graupel due to the riming.

FREEZING AND MELTING Previously, it has been discussed that freezing of cloud droplets can occur in different ways. In the case of raindrops, only heterogeneous freezing plays a role as the raindrops freeze before reaching the temperature regime where homogeneous freezing occurs. In SB06, the frozen hydrometeors classes are separated by size, so the size of the frozen raindrop will decide if the amount of ice, graupel or hail will increase. Such freezing processes may produce secondary ice particles due to the mechanical stress which the newly formed ice surface undergoes (Lauber et al., 2018). In cases where frozen hydrometeors exist and the surrounding air temperature increases, melting can occur. As this will not directly convert the frozen hydrometeor into liquid, a characteristic time for melting is used. Further, evaporation may occur above the now liquid surface, which is also parameterised.

WEGENER-BERGERON-FINDEISEN PROCESS The Wegener-Bergeron-Findeisen process (WBF; Bergeron, 1935; Findeisen, 1938; Wegener, 1911) is not a separate microphysical process but describes the interaction of evaporation and deposition in mixed-phase regions. As mentioned before, the saturation vapour pressure with respect to ice $e_{s,i}$ is lower than the saturation vapour pressure with respect to water $e_{s,w}$. This means an air parcel may be supersaturated with respect to ice $S_i > 1$ while it is unsaturated with respect to water $S_w < 1$. This can cause deposition to occur simultaneously with evaporation in MPCs. The deposition of water vapour causes a further decrease in the saturation, causing even more evaporation from surrounding water droplets. The water vapour formed by the evaporation can now be deposited on the ice particles, which have grown further while the droplets have decreased in size. This phenomenon is difficult to capture correctly in large-scale models, as the homogeneous distribution of ice and supercooled liquid in a single grid box can quickly cause the full glaciation of the clouds in that grid box (Huang et al., 2021; Storelvmo, Tan, and Korolev, 2015). In reality, though, the supercooled liquid in an inhomogeneously mixed cloud can be spatially separated from the ice (Korolev et al., 2017). For example, in the form of liquid layers in Arctic low-level stratiform clouds. Based on theoretical calculations Korolev (2008) describes two vertical velocity regions in which the WBF causes the growth of ice at the cost of liquid droplets. Generally, the WBF process does not occur for upward and strong downward velocities. Additionally, the air must be saturated with respect to ice but not to water, which is another limiting factor.

4 DATA AND IMPLEMENTED TOOLS

This chapter describes the data and implemented tools which were used to produce the results presented in the chapters 5, 6 and 7. First, the observational data sets are presented. Secondly, a description of the daily workflow of the ICON simulations, which was set up for this thesis, is provided. In the third section, the microphysical wrapper, used to acquire the microphysical process rates, is described, and some test results are shown.

4.1 OBSERVATIONAL DATA AND DERIVED DATA PRODUCTS

In this dissertation, observational data is used to evaluate the model data. The instruments providing this data are located in Ny-Ålesund. They are maintained by the German-French AWIPEV research base that is operated jointly by the Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research (AWI) and the French Polar Institute Paul Emile Victor (IPEV). AWIPEV is part of the Ny-Ålesund Research Station and is operated year-round. The instruments and derived products which were used here are the radiosondes, the microwave radiometer (MWR) HATPRO, Cloudnet and the rain gauge Pluvio.

THE MICROWAVE RADIOMETER HATPRO (HUMIDITY AND TEMPERATURE PROFILER) is a passive instrument (Rose et al., 2005). It measures the brightness temperature T_b from which the temperature and humidity profile, the integrated water vapour (IWV), and the liquid water path (LWP) can be derived. It measures on 14 channels in two bands, 22-31 and 51-58 GHz, with a measurement frequency of 1 to 2 seconds. The retrieval for the IWV and LWP are based on Löhnert and Crewell (2003) and were adjusted based on Nomokonova et al. (2019) for Ny-Ålesund. For higher values, the accuracy of the measured IWV decreases when compared to radiosonde data, also for the location-adjusted version (Kiszler, Ebell, and Schemann, 2023). Cases where there is rain or when the radome is wet are unreliable and therefore flagged and excluded from the analysis. In cases where the data from HATPRO is compared to simulation data, the flagging of the data is mimicked by setting a rain threshold above which simulation data will not be used. This is mentioned accordingly in each study where this is done. With an accuracy of $\pm 20 - 25$ g m^{-2} for the

Figure 3: Cloudnet classification for Ny-Ålesund showing the 10 classification categories based on the combination of observational and weather prediction model data in the upper panel. The bottom panel shows the data availability. Case: 12.08.2023, Source: *University of Cologne Quicklooks* (Accessed: 10.10.2023).

LWP (Rose et al., 2005), thin liquid clouds or cloud layers are hard to detect and make a comparison to the model slightly challenging.

CLOUDNET The Cloudnet product introduced by Illingworth et al. (2007) was developed to simplify the comparison of observation and model data. It provides a target classification based on a combination of remote sensing instruments and a numerical weather prediction model to achieve this. The Cloudnet data in this work was created using a combination of the AWI Ceilometer CL51 and the University of Cologne 94 GHz cloud radar JOYRAD-94, as well as ICON-NWP (temperature, humidity, and pressure). The target classification includes 10 different categories. These are aerosols, aerosols & insects, insects, droplets, ice, drizzle or rain, melting & droplets, melting ice, drizzle & droplets, and ice & droplets (Example in Figure 3). A model version of Cloudnet was produced to compare this data with ICON. For this, the categories have been reduced to five categories and only include hydrometeors. These categories are cloud droplets, drizzle or rain, drizzle/rain & droplets, ice & snow & graupel, and ice & droplets. The categories are based on a threshold of 10^{-8} kg kg^{-1} for the mass mixing ratio and are defined as logical conditions. An example of how the output looks is shown in Figure 3 and Figure 4 for a single day at AWIPEV.

RADIOSONDES The radiosondes used in this dissertation are Vaisala RS41 radiosondes launched daily at 1200 UTC. The radiosondes belong to the GRUAN network (Global Climate Observing System Reference Upper-Air Network) and measure the temperature, relative humidity, wind speed and direction, and pressure. A more in-depth background of the radiosonde data is given in Maturilli and Kayser (2017).

Figure 4: Cloudnet classification for Ny-Ålesund showing the five categories based on the ICON-LEM data. Case: 12.08.2023, Available online: *University of Cologne Quicklooks* (Accessed: 10.10.2023).

RAIN GAUGE PLUVIO The University of Cologne's Pluvio precipitation gauge is used to measure the precipitation. This instrument is produced by the company OTT and is constructed as a cylinder in which the precipitation should fall and where the amount is weighed and given as accumulated precipitation for each minute. The measurement threshold is given as 0.1 mm within a minute or 0.05 mm within an hour. One problem with such precipitation gauges is that they can miss precipitation which does not fall into the cylinder, for instance, due to turbulence. Strong winds can further cause massive differences in what is measured compared to what actually fell, especially when it comes to snow (Førland and Hanssen-Bauer, 2000). As snow is common in Ny-Ålesund, corrections are available to account for the wind-induced loss. These include those by Førland and Hanssen-Bauer (2000), Wolff et al. (2015), and Kochendorfer et al. (2017).

4.2 A SEMI-OPERATIONAL SIMULATION SETUP

A crucial piece of this thesis is the simulation data which is used for the analysis. A large proportion relies on data from a semi-operational ICON simulation workflow (Figure 5), which was set up early on as part of this work. These 24 hr simulations ran automatically on a daily basis and are centered around Ny-Ålesund. They consist of two limited area simulations, one with 2.4 km and one with 624 m resolution. The forcing data needed for these limited area simulations is taken from the operational global ICON-NWP forecast with 13 km resolution. Each day a subset of the global forecast covering the Fram Strait and Svalbard is provided by the German weather service (Deutscher Wetterdienst, DWD). In the first step of the workflow, this 13 km data is remapped to a smaller grid with a cell size

of 2.4 km (Figure 5 step 1). ICON is then run for the 2.4 km resolution domain in the ICON-NWP mode starting at 00:00 UTC. After this has succeeded, the data of the 2.4 km simulation is remapped to a simulation domain with 624 m resolution (Figure 5 step 2). The second simulation is then run on the 624 m domain in the LEM mode, also starting at 00:00 UTC (Figure 5 step 3). As shown in Figure 5 step 4, the ICON-LEM output is further processed and visualizations for certain variables are created automatically. For the topography, the GLOBE dataset with around 1 km resolution is used, although, in the future, one could consider a switch to the more finely resolved MERIT-DEM dataset, which has become available recently in ICON. In Section 3.1, it is discussed that the effective resolution of ICON-LEM has been shown to be around eight times the cell size (Heinze et al., 2017; Zängl et al., 2015). It was further mentioned that the triangular edge length (resolution) can be approximated as $2/3\overline{\Delta x}$ in square edge length. The given triangular edge length of 624 m corresponds to a square edge length $\sim$ 416 m. Therefore, the chosen resolution lies in an area which is very finely resolved for a NWP model but not enough for an LEM and is in the "grey zone" of resolved turbulence (Honnert et al., 2020). Because no grey zone parameterisation is currently available in ICON for turbulence, one has to decide between ICON-LEM or ICON-NWP. This is not the first time, though, that studies have been confronted with this issue in ICON, and several studies have provided good results using ICON-LEM in the grey zone (e.g. Heinze et al., 2017; Ori et al., 2020; Schemann, Ebell, et al., 2020). Indeed, comparing ICON-LEM simulations with around 600 m resolution to finer resolved ICON-LEM simulations showed that the general cloud structure could already be well captured with 600 m resolution (Schemann and Ebell, 2020; Schemann, Ebell, et al., 2020). These findings of previous studies encouraged running the simulations with around 600 m resolution. This allowed for the performance of daily simulations, which would not have been the case for higher resolutions where the computational cost increases significantly. Further details regarding the simulation setup are explained in the publication included in chapter 5.

One setting which is worth mentioning is a switch of the nucleation and activation schemes in the simulations. This switching of the INP nucleation and CCN activation, undertaken in May 2021, strongly impacted the cloud hydrometeor composition (see Chapter 6). For several months two ICON-LEM setups were running in parallel, one with the default activation settings and the second with the changed activation setting. In the default version, continental aerosols are used as described by Hande et al. (2016, CCN) and Hande et al. (2015, INP). In the newer version, the CCN activation by Segal and Khain (2006) and the INP nucleation by Phillips, DeMott, and Andronache (2008)

Figure 5: Schematic of the daily ICON simulation workflow demonstrating the individual steps. Only an excerpt of the ICON-NWP 13 km global simulation is shown in the top figure. The colourbar for the topography is identical for all maps. The lowest figure is an example of a PAMTRA forward simulation taken from the *University of Cologne Quicklooks* (Accessed: 10.10.2023).

were used. Three aerosol types were available for the nucleation, but only initial dust was included in these simulations. In Chapter 6, an overview of the impacts of these changes is presented.

The results of this thesis build on the accumulated set of simulations, and substantial effort was invested to provide these simulations as continuously as possible. Several changes to the output settings were made to adapt the setup to the needs of other researchers during certain periods. Publicly available plots showing the IWV, LWP, IWP, Cloudnet classification, and forward simulations using the Passive and Active Microwave TRAnsfer model (PAMTRA; Mech et al., 2020) can be found online (*University of Cologne Quicklooks* Accessed: 10.10.2023, Time period beginning 01.08.2020). These simulations have also benefited others and have been, for instance, used by Chellini et al. (2023) to support an observational data set.

4.3 EXTRACTING MICROPHYSICAL PROCESS RATES

The second tool, which was developed and implemented, is a Fortran wrapper enabling users to run the two-moment microphysics scheme by Seifert and Beheng (2006) (see Section 3.2) independently of the ICON model to output the process rates of all microphysical processes. In the context of the before mentioned general kinetic microphysics Equation 4, this means the interest here lies in the rates of the microphysical processes $P_1, P_2, ...P_N$. The advection and sedimentation of the hydrometeor are not considered in this approach. The wrapper functions as an interface to use the microphysical parameterisation in a diagnostic manner. The schematic in Figure 6 demonstrates the concept. There are several reasons why this is advantageous in comparison to directly outputting the microphysical tendencies from the model:

1. It is extremely fast to run single columns or timesteps, and it saves the time used to write the full output during the simulation as well as reprocessing time.

2. It reduces the output data amount massively, as one can refine for which cell/column/area, timesteps and processes the output should be created.

3. Changes in the microphysical parameterisation can undergo a quick check to see how they might impact the full ICON simulations.

Obviously, this also entails some limitations:

1. The computed hydrometeor mass will not be the same as in the model, as the transportation between cells is not included.

Figure 6: Simplified schematic of the two-moment microphysics parameterisation wrapper demonstrating the underlying concept. The purple box shows the adapted SB06 code taken from the ICON model. Green boxes show parts of the code which only belong to the wrapper.

2. It cannot show the full impact of a change to the microphysical code, as each timestep relies solely on the original simulation output and is not informed by the previous steps.

The following section provides an overview of the implementation of the wrapper, and a short evaluation of the impact of advection and sedimentation is given.

4.3.1 *Implementation*

The wrapper, which is implemented in FORTRAN with additional post-processing scripts in Bash and Python[1] is built in a way that it mimics the interface where the two-moments microphysics are called. To achieve this, one must provide the same input as done in the model (see Appendix Table 2). Therefore, one of the first steps is to read the provided ICON output files and store the thermodynamic and hydrometeor variables. The input file paths are provided by namelists, in which one can also define whether the data is either 3D or 2D input. This makes a difference in the way the data is allocated. 3D data will further be split into slices if it is larger than the threshold given in the namelist variable `max_ncells`. This is necessary if one wants to

1 The code is available on the German climate computing centre (DKRZ) Gitlab, but currently can only be accessed by those who have an ICON-licence. This is due to the fact that ICON code is incorporated, which is not open-source.

run the wrapper using 3D input data while constraining the computational burden and required memory.

After setting all variables, the two-moment microphysics scheme is initialized. Then, the saturation adjustment and microphysics scheme are called. This is done using the pressure, density, temperature, and vertical wind from the current timestep and the hydrometeor values from the previous timestep. Different timesteps must be chosen because the system would be in equilibrium otherwise, as the output of the model is used, which is the equilibrium state at a current timestep. The saturation adjustment is called once before and once after the two-moment microphysics scheme in ICON. Therefore, the same is done in the wrapper.

For each timestep, the process rates are added to the output. The process rates are given as the differences between each hydrometeor mixing ratio before and after a process is called. Technically, they are first computed as the difference of the hydrometeor mass densities, but they are converted into the difference in mass mixing ratios to match the hydrometeor mass mixing ratios. A summary of the main steps is given in Figure 6. The output contains the updated hydrometeor masses and their tendencies (Appendix Table 3). For each process, at least two hydrometeor types must be affected as the mass must be conserved. For some, several hydrometeor types are impacted, and sometimes the mass change can be either positive or negative, for instance, for evaporation and condensation.

4.3.2 *Microphysical processes vs. transportation*

This section shows some results of the tests conducted to see how much mass changes are captured by the wrapper approach. This gives an estimate of how much of the mass change is due to the microphysics and how much is due to advection and sedimentation. It is expected that there should be differences in the wrapper mass output in comparison to the original output as the wrapper only runs the microphysical parameterisation and saturation adjustment in each step. To achieve an estimate, the difference in the hydrometeor masses between the wrapper and the actual simulation output was evaluated. The case used here consists of the first three hours of 04.10.2022, which cover a mixed-phase cloud that contains all hydrometeors except hail. This simulation was run with a Meteogram output frequency and model timestep of 3 seconds. The analysis was then limited to the cloudy pixels (mass $> 10^{-8}$ kg kg^{-1}), for which one can see that the relative difference does not depend on the actual mass. This can be seen in Figure 7, which shows the absolute difference against the original mass and the colour-coded relative dif-

ference. In Figure 7, one can further see that the majority of the points lie below a relative difference of 10%. The maximum difference was found for the cloud droplet mass and lies at $7 \cdot 10^{-6}$ kg kg^{-1}. It further makes sense that the precipitating hydrometeors (Figure 7 a, c, e) have slightly higher relative differences in comparison to cloud ice and cloud droplets (Figure 7 b, d). This is because one can expect sublimation to play a larger role for the larger hydrometeor types. The small relative difference shows that a large fraction of the mass change can be explained by purely evaluating the microphysical process rates in cases where no strong transportation is expected.

To reduce the amount of data, the model output used throughout this dissertation was downscaled to every 9 seconds while the time integration still had a timestep of 3 seconds. For the 9-second output, it was also found that the microphysical processes strongly dominate the hydrometeor mass changes. Another consideration was whether the use of the thermodynamical variables from 3 timesteps back instead of 1 would be an issue. The case used to perform the tests did not show a large difference, though, and the number of cases remained in the same range. Therefore, the 9-second output in the meteogram is sufficient to study the microphysical processes.

Figure 7: Absolute difference of the wrapper and original simulation plotted against the original mass simulated by ICON-LEM. The hydrometeors are a) graupel, b) cloud droplets, c) rain, d) cloud ice and e) snow. The data includes 3 hours with a timestep of 3 seconds on 150 levels. The number of occurrences per bin is colour-coded, but as the ranges are different, the subplots use different colour-bar ranges. The red dashed lines indicate the relative differences of 10% and 1%.

Part III

STUDIES

5

A PERFORMANCE BASELINE FOR THE REPRESENTATION OF CLOUDS AND HUMIDITY IN CLOUD-RESOLVING ICON-LEM SIMULATIONS IN THE ARCTIC

The first study addresses the question of to what extent the ICON model can capture the thermodynamical and macro-scale cloud processes in the Arctic. For this purpose, the focus lies on Ny-Ålesund, which presents a complex environment whilst providing a wealth of observational instruments. This study has been published, reference below, and is therefore included in the journal layout.

Kiszler, T., Ebell, K., & Schemann, V. (2023). **A performance baseline for the representation of clouds and humidity in cloud-resolving ICON-LEM simulations in the Arctic**. Journal of Advances in Modeling Earth Systems, 15, e2022MS003299. https://doi.org/10.1029/2022MS003299

Author contributions: TK set up and ran the simulations, analysed and visualised the data, and created the original manuscript, which all authors reviewed and edited. VS and KE provided scientific supervision and helped with the conceptualisation. VS supported the simulation setup, and KE provided support for the observational data analysis.

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RESEARCH ARTICLE
10.1029/2022MS003299

Key Points:

- Cloud resolving simulations for several months using the ICOsahedral Non-hydrostatic model Large-Eddy model in the Arctic are evaluated
- High agreement of model and observations on wind flow, integrated water vapor, and light to medium precipitation
- More clouds are simulated than observed but at the same time the model clouds lack liquid water

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A Performance Baseline for the Representation of Clouds and Humidity in Cloud-Resolving ICON-LEM Simulations in the Arctic

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Abstract In the context of Arctic amplification many of the feedback mechanisms, decreasing or enhancing the warming, involve clouds and water vapor. Currently, there is a gap in understanding the role of clouds which leads to uncertainties in climate simulations. Modeling frameworks such as the ICOsahedral Non-hydrostatic model (ICON) are used to understand the Arctic atmospheric processes as well as predict future changes. In this study, we challenge ICON in the large-eddy setup (ICON-LEM) by performing cloud-resolving simulations over parts of Svalbard, including Ny-Ålesund. We ran daily simulations over 5 months and analyzed the column above Ny-Ålesund. The local supersite's observations enabled us to create a baseline for the model performance focusing on the representation of liquid water and water vapor. We narrow in on possibilities to improve the cloud microphysical representation based on statistical evaluations, not just single cases. We found an astonishing agreement between most of the analyzed variables. For instance, the model integrated water vapor showed only a low bias of 0.21 kg m^{-2}. The number of cloudy days is slightly higher in the model (+4%). Further, we found that the model produces an unrealistically high number of pure ice clouds. Small to medium precipitation events are similar in amount and time but the number of strong precipitation events is underestimated. Further results are discussed and show that ICON-LEM is a useful tool to study the Arctic. With this thorough analysis, we highlight the value of local cloud-resolving simulations to understand changes in the Arctic atmosphere.

Plain Language Summary The Arctic is warming faster than the rest of the globe. Many atmospheric processes impact the rate of the warming. Explaining these processes is challenging. Especially processes involving clouds lack sufficient understanding. We can use computer models to answer some of our questions, but for that, the models must be good enough and we must know their limitations. In this study, we used several months of simulations for Svalbard which we created with the ICOsahedral Non-hydrostatic (ICON) model. The simulations had a high resolution and we used a model specialized for that: The ICON Large-Eddy model (ICON-LEM). We analyzed how well the model can represent clouds and humidity. One result is that many clouds contained more ice than what was measured at that location. We also found that the model produced more clouds than were observed. On the other side, the water vapor amount and wind field were simulated relatively precisely. The results show that the ICON model is helpful to study the Arctic. The ability to analyze many cases made it possible to quantify some of the limitations in the creation and development of clouds and precipitation. Knowing these limitations will help us to improve the model in the future.

1. Introduction

The current Arctic amplification is determined by many processes which interact with each other. The warming is approximately taking place two to four times as fast as the average global warming (Hahn et al., 2021; Post et al., 2019; Serreze & Barry, 2011). Additionally, there is a pronounced seasonal dependence with the largest temperature anomalies in winter. It is further noticeable that the temperature increase is not equally distributed over the Arctic, and some regions such as the Svalbard Archipelago are more strongly affected (Dahlke & Maturilli, 2017; Jansen et al., 2020). On the Svalbard Archipelago long-term observational stations such as in Ny-Ålesund have been providing data for several decades showing the changes in atmospheric variables (Førland et al., 2011; Maturilli & Kayser, 2017). The Ny-Ålesund measurement site and its surroundings' representation of the greater Arctic are disputable due to the intricate topography and heterogeneous surface types. Nevertheless,

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it provides a large data collection analyzed in numerous studies (e.g., Argentini et al., 2003; Gierens et al., 2020; Maturilli et al., 2013; Nomokonova et al., 2019; Vihma et al., 2011).

Feedback mechanisms, which may either increase or decrease the warming, are manifold and their impacts and interactions are difficult to quantify (Goosse et al., 2018). Several of these feedback mechanisms involve water vapor and clouds. Clouds impact the radiation budget and changes in cloud cover, optical thickness or the phase composition can have both warming and cooling effects. Current climate models reveal that the cloud feedback is possibly of smaller importance (Block et al., 2020; Pithan & Mauritsen, 2014). However, these models are still prone to large uncertainties in the representation of clouds resulting also in large uncertainties in climate prediction. These uncertainties stem from insufficient process understanding and the misrepresentation of clouds in models and make climate predictions vary widely (Schneider et al., 2017). Kay et al. (2016) discusses the connection of these knowledge gaps with challenges in measuring the cloud properties on large and small scales accurately.

Water vapor is another crucial variable and there is a clear positive feedback of water vapor versus the downward longwave radiation flux (Ghatak & Miller, 2013). Long-term trend analyses, such as in Rinke et al. (2019) which showed the consistent moistening of the Arctic over two decades, are important from a climate perspective. But measuring water vapor with high spatiotemporal resolution in the Arctic is difficult. Satellite retrievals provide helpful data but are biased and can show large differences depending on the product (Crewell et al., 2021). Dedicated campaigns in the Arctic such as Multidisciplinary drifting Observatory for the Study of Arctic Climate (Shupe et al., 2022), Arctic CLoud Observations Using airborne measurements during polar Day (Wendisch et al., 2019) or Surface Heat Budget of the Arctic Ocean (Uttal et al., 2002), provide more detailed data with the disadvantage of being limited in area and time. On the other hand, supersites, such as Ny-Ålesund (Svalbard), provide long-term and continuous observations of the Arctic atmosphere. This is necessary to establish changes in the local climate. A study by Maturilli and Kayser (2017) for instance, analyzing the radiosonde measurements from Ny-Ålesund for two decades, showed the increase of integrated water vapor (IWV) during the winter, which generally is the season with the lowest humidity.

In light of the lack of high-quality observations in the Arctic, models can help to support the analysis and close some of the gaps. One of these models is the ICOsahedral Nonhydrostatic model (ICON) which has been primarily developed for the mid-latitudes. This model consists of a non-hydrostatic dynamical core (Zängl et al., 2015) and can be used with different modules for climate simulations, numerical weather prediction, and large-eddy simulations (Dipankar et al., 2015). For the mid-latitudes ICON is a reliable and tested model although, as in other models (Morrison et al., 2020), clouds and precipitation remain persistent challenges. This could also be seen in the highly resolved ICON-LEM simulations performed over Germany by Schemann et al. (2020) and Heinze et al. (2017). Deficiencies in the micro-physics schemes implemented in ICON have been pinpointed in other studies as well (Karrer et al., 2021; Kretzschmar et al., 2020; Ori et al., 2020). As interest in the Arctic environment has been growing, ICON has been used for the higher latitudes in different setups for case studies and campaigns (Bresson et al., 2022; Gruber et al., 2019; Wendisch et al., 2019). Schemann and Ebell (2020) performed high-resolution simulations using ICON-LEM for several days focusing on a small domain around Ny-Ålesund. They showed that the model can capture local humidity variability and is capable of representing the mixed-phase clouds although deficiencies in the microphysical parameterization are also discussed. They further explored the benefits of using resolutions up to 75 m. The work presented here can be seen as a more detailed and expanded extension of this.

It is clear that to better understand and predict the atmospheric processes in the Arctic, we must know how well the models can represent them. Only if this is the case we can effectively work on improving the models not just for single cases. ICON has not yet been evaluated for a large set of cases covering a diverse range of synoptic events in the Arctic. For this reason, we set up a semi-operational workflow and ran daily cloud-resolving simulations for a complex domain in the Arctic. The setup is described in Section 2.1. Using the super-site location Ny-Ålesund we were able to exploit a variety of observational data (Section 2.2). The results of the evaluation using 5 months of these daily simulations can be found in Section 3. First, we evaluate the performance of the model exploring the impact of the topography on the flow (Section 3.1) and then focus on the typical modeling weak spots; clouds, humidity, and precipitation (Sections 3.2–3.5).

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Figure 1. Domains used for the ICOsahedral Non-hydrostatic model (ICON) simulations. The white domain marks the outer domain used for ICON-numerical weather prediction model with a resolution of 2.4 km. In this domain, the topography is shown in greyscale. The circular domain, centered at Ny-Ålesund is used in ICON-Large-Eddy model with a resolution of 600 m.

2. Methods and Data

2.1. The ICON Model and Simulation Setup

The ICOsahedral Non-hydrostatic (ICON) unified modeling framework was originally developed by the German Weather Service and Max-Plank Institute for Meteorology. We used the ability of the model to run as a numerical weather prediction model (ICON-NWP) as well as a large-eddy model (ICON-LEM). This enables consistency throughout the workflow as the dynamical core of ICON is the same for both versions. The differences lie in the parameterizations of sub-grid scale processes such as turbulence and cloud fraction (Dipankar et al., 2015). Further, in ICON-NWP we use 150 vertical levels versus 100 levels in ICON-LEM, as the higher resolution is computationally more expensive. Both setups use the hybrid Smooth LEvel VErtical coordinates SLEVE (Leuenberger et al., 2010; Schär et al., 2002) with the layer thickness for ICON-LEM increasing from 20 to 140 m in the lowest 3 km. One reason why Ny-Ålesund is challenging is that the topography plays an important role in the mountainous area of Svalbard. Following the assumption that the resolution is fine enough to resolve the impact of the orography on the flow, the parameterization of sub-grid scale orographic drag is turned off. The radiation is computed using the Rapid Radiative Transfer Model (Barker et al., 2003; Mlawer et al., 1997) in both setups. Continuing with further differences, the cloud-resolving grid in ICON-LEM makes it possible to use an all-or-nothing scheme for the cloud cover. In ICON-NWP this is computed using a diagnostic PDF (Köhler et al., 2011). In ICON-NWP the convection still relies on the parameterization by Tiedtke (1989) and Bechtold et al. (2008) but is turned off in ICON-LEM. Fundamental to the value of the large-eddy simulations is the 3D Smagorinsky scheme used for turbulent diffusion in comparison to the prognostic TKE computation implemented for ICON-NWP. Further, the use of the two-moment cloud microphysics scheme by Seifert and Beheng (2006) enables a better representation of the cloud micro-scale processes in ICON-LEM in contrast to the single-moment scheme used for ICON-NWP.

Our workflow consisted of two simulations for each day. The first simulation, with 2.4 km resolution, used ICON-NWP and the second, with 600 m resolution, ICON-LEM. The simulation setup used by Schemann and Ebell (2020) for ICON-LEM was adopted for this purpose.

Here we focus mainly on the results of the simulations using ICON-LEM. In two cases the ICON-NWP results are included to highlight improvements of the ICON-LEM but also to show when 2.4 km can be a sufficient choice. As can be seen in Figure 1 the domain for ICON-LEM only covers a limited circular area with 110 km diameter centered around Ny-Ålesund and including the neighboring fjord Kongsfjorden. Therefore, it was necessary to provide forcing data. For this, we acquired data from the daily global operational ICON simulations, performed by the German Weather Service with a resolution of 13 km. Remapping the 13 km data to 600 m is not ideal due to the large resolution jump. Hence, we decided to additionally run ICON-NWP with 2.4 km resolution for a limited domain covering most of Svalbard and including parts of the Arctic Ocean surrounding the archipelago. These intermediate simulations were forced using the ICON global simulations and the output was remapped to force the ICON-LEM runs. Both simulations were initialized at 00:00 UTC and simulated a 24 hr period. For the analysis, the first 3 hr were excluded to avoid the spin-up period.

The simulation set used for this study includes all available daily simulations from August to December 2020. During this period the fjord remained ice free. Only some variables are stored as this enables us to use a very high temporal resolution of 9s. This subset is a Meteogram containing the output of a single column. For our purposes, the Meteogram for the grid-cell in which the Arctic Research Base "AWIPEV" (see next section) in Ny-Ålesund is located, is returned.

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Table 1
Instruments and Data Sets Used in This Study

Data source	Variables	Temporal resolution	Specifications
MWR HATPRO	IWV, LWP	1–2 s	22–31 and 51–58 GHz
Cloudnet	Target classification	30 s	Input: Ceilometer CL51, 94 GHz cloud radar, ICON-NWP
Radiosondes	Temperature, relative humidity, and wind direction	Daily, 12:00 UTC	Vaisala RS41
Rain gauge Pluvio	Accumulated precipitation	60 s	

2.2. Observations and Data Processing

The observations for Ny-Ålesund are obtained from the before mentioned AWIPEV station. An overview is given in Table 1. The data that we used include the daily operational 12:00 UTC radiosondes (Maturilli, 2020) which are typically launched around 11:00 UTC. The lowest 100 m have larger uncertainties because the radiosondes are closer to the balloon while the attachment cord is still unraveling. For the comparison between the radiosondes and the simulations, only a subset of the model data was used. Depending on the variable evaluated, either the 12:00 UTC Meteogram was selected or the average of the Meteograms from 11:00 to 11:20 UTC was taken. This is mentioned accordingly in the results. The precipitation is measured by the University of Cologne's Pluvio precipitation gauge. Several corrections following Wolff et al. (2015), Førland and Hanssen-Bauer (2000), and Kochendorfer et al. (2017) have been applied to the original Pluvio data to account for wind-induced loss and give an idea of the uncertainty of the observed precipitation estimate.

2.2.1. The Humidity and Temperature Profiler HATPRO

The vertically integrated cloud water (liquid water path [LWP]) and IWV are taken from the Humidity And Temperature PROfiler (HATPRO) of the Alfred Wegener Institute for Polar and Marine Research (Ebell & Ritter, 2022). HATPRO is a passive microwave radiometer (MWR) providing brightness temperature measurements at 14 frequencies in two different spectral bands with a temporal resolution of about 1 s. Based on these brightness temperatures, LWP and IWV have been retrieved (Nomokonova et al., 2019). Uncertainties for LWP are typically 20–25 g m^{-2} and for IWV smaller than 1 kg m^{-2}. The data is interpolated to 1-min values for the comparison with the model data. In this analysis, the measurements have been discarded in cases where the quality flag indicated precipitation. The precipitation is registered by a sensor on the instrument. Precipitation might result in a wet radome, leading to erroneous LWP and IWV estimates. A blower prevents the deposition of snow on the instrument. An additional check was applied to exclude times when the MWR brightness temperatures of one frequency channel were spectrally inconsistent with the other channels of the same band. To compare the observed LWP and IWV to the model we applied an artificial flagging in the model data as well by excluding all time periods where liquid precipitation is above 0.05 mm in the model. This leads to a justifiable comparison but one must keep in mind, that it is still likely that cases remain in the model data which would be excluded in the observational set.

2.2.2. Separating Cloudy and Clear Columns

To distinguish between cloudy and clear columns the Cloudnet data products were used. Cloudnet was specifically developed by Illingworth et al. (2007) to facilitate the operational evaluation of clouds in NWP models using ground-based observations. In particular, the Cloudnet target classification product enables the user to differentiate between water in different phases, aerosols, and other non-hydrometeors in the cloud radar height bins. The column height reaches up to 12 km.

To create this target classification, several ground-based remote sensing instruments are combined. For AWIPEV, this includes the AWI Ceilometer CL51 and the University of Cologne 94 GHz cloud radar JOYRAD-94. The Cloudnet target classification also needs thermodynamic information (temperature, pressure, and humidity profiles) which is taken from the ICON-NWP global operational runs (13 km resolution). For the ICON-LEM data, the creation of such a target categorization is done by applying thresholds to the hydrometeor concentrations of the different particles (ice, cloud droplet, raindrop, graupel, and hail). For this, a common threshold of 10^{-8} kg kg^{-1} was applied to the concentrations in the columnar output of the Meteogram (Schemann & Ebell, 2020).

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Figure 2. Occurrence of wind direction with height taken from the (a) radiosondes, (b) ICOsahedral Non-hydrostatic model Large-Eddy model (ICON-LEM) and (c) ICON-numerical weather prediction model (NWP) profiles (August to December 2020). The wind direction is binned in 10° steps. The heights in ICON-NWP and the radiosondes are adapted to the ICON-LEM levels. The radiosondes were started around 11:00 UTC and from the simulations, a single profile at 12:00 UTC was selected. The gray dashed lines indicate the level at 180 m.

3. Results and Discussion

3.1. Boundary Layer and Free Atmospheric Flow

As mentioned before, the terrain around Ny-Ålesund provides the opportunity to test the capability of the model to capture the flow in the boundary layer (BL) and free troposphere. Both can be distinguished very clearly from each other and the sea-land breeze, as well as katabatic winds in the fjord, are well-studied phenomena (Beine et al., 2001; Esau & Repina, 2012; Vihma et al., 2011). The radiosondes from 1993 to 2014 analyzed by Maturilli and Kayser (2017) show the southeast low-level flow which is channeled through the fjord (see Figure 1 in Maturilli and Kayser (2017)). At roughly 1 km height the impact of the topography has decreased so far that the flow begins to rotate toward a south-westerly flow, which then dominates in the free troposphere. Reassuringly, both aspects of the flow can be seen very clearly in the ICON-LEM and ICON-NWP simulations. To depict this in Figure 2 only the 12:00 UTC profiles from the simulations were used. The radiosonde profiles were used as reference. The height bins are computed using the lowest vertical resolution of the three data sets which is the ICON-LEM, as these simulations only have 100 model levels in total. For the wind direction, 10° bins are used. The advantage of using the higher resolved simulation becomes clearer when looking at single layers in the BL. The smoothed distribution of the wind direction for the fifth model level (≈180 m) is shown in Figure 3. The maxima are underestimated in both model versions but the higher resolved simulations capture the accumulation around 110° more accurately, although it is slightly shifted southwards. The higher accuracy for the ICON-LEM simulations makes sense as the higher resolution can resolve more of the flow and has a better representation of the topography. As the topography input is limited in resolution we can see though that for other study purposes the 2.4 km resolution of ICON-NWP may be sufficient regarding the wind flow. Here ICON-NWP too captures the main features of the flow accurately.

Figure 3. Frequency of occurrence of wind direction taken from the radiosondes (black dashed), ICOsahedral Non-hydrostatic model Large-Eddy model (red solid) and ICON-numerical weather prediction model (blue dashed-dotted) profiles (August to December 2020) for the single level at a height of ca. 180 m. The model data consists of single profiles at 12:00 UTC.

Another phenomenon of the BL around Ny-Ålesund are the orographically induced waves. We were able to observe these in the model (not shown). These waves occur when the air masses overflow the mountains to the south of Ny-Ålesund. In some of the simulations they led to high vertical winds (>4 m s^{-1}) and typical wave patterns in the wind signal. Understanding how they influence clouds would need further research.

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Figure 4. Mean vertical profile of (a) temperature, (b) specific humidity, and (c) relative humidity for ICOsahedral Non-hydrostatic model Large-Eddy model (ICON-LEM) (solid red) and radiosondes (dashed black) from August to December 2020 below 2.5 km. The shaded areas show the interquartile ranges (IQR; red: ICON-LEM, gray: Radiosondes).

3.2. Boundary Layer Profiles

3.2.1. Temperature and Humidity

The representation of the vertical profiles in the lower levels plays an important role for the low-level clouds in the model. Therefore, we investigated the temperature and humidity using the daily soundings. The model is able to capture the general structure of the temperature and humidity profiles well. Figure 4 depicts a close-up of the mean profiles below 2.5 km with the interquartile ranges. It is noticeable that there is on average a cold bias of −0.37 K in the model throughout the troposphere (below 10 km). The bias increases toward the surface and reaches—1.33 K at 130 m (Figure 4a). Nomokonova et al. (2019) found that this negative bias in the BL was even stronger in ICON-NWP global simulations with 13 km resolution.

Concerning the humidity, one can see an underestimation of specific humidity in the model which increases toward the surface (Figure 4b). The cold bias on the other side balances out the lack of humidity and consequently, the mean relative humidity profiles agree well (Figure 4c). A relative humidity inversion can be seen around 100 m which is slightly more pronounced in the observations mean than in the model mean. Between 0.5 and 1.5 km, ICON-LEM is on average drier but has a larger spread. This is the layer where the majority of the low-level mixed-phase clouds develop.

3.2.2. Relative Humidity Modes

When one now expands the view to include the variability of the relative humidity in each level an interesting feature becomes visible in the observations. As depicted in Figure 5, the radiosondes show a bi-modal distribution of the relative humidity up to a height of 1 km. Especially between 500 m and 1 km, this is visible. When looking at the simulations only one mode is visible. This feature is not restricted to specific seasons and is connected to the drift of the radiosondes. To show this, the trajectories were split into two groups. As the criterion, the mean relative humidity between 500 and 600 m is selected. In this height range, the two modes can be distinguished well from each other. In Figure 6 the histogram makes the two modes visible and based on the distribution a threshold of 87% relative humidity is chosen to distinguish the two sets. Using this the trajectories are visualized in Figure 7 where it becomes clear that the majority of the mode with the higher relative humidity stems from drifts toward and over the fjord.

This gives some insights into the spatial variability of the humidity in the local area around Ny-Ålesund. The evaporation from the fjord seems to cause a higher humidity over the fjord. It further highlights the necessity for caution when comparing the single-column output of a model with non-stationary observational sets. Here, large

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Figure 5. Frequency of relative humidity with height for (a) ICOsahedral Non-hydrostatic model Large-Eddy model and (b) the radiosondes (August to December 2020). The gray dashed lines mark the 500 and 600 m levels.

differences between the model and the radiosondes can partially be explained by the trajectory of the radiosonde. Therefore, studies containing only a single or few cases must take this into account.

3.3. Integrated Water Vapor

In this section, we analyze the capability of the model to accurately capture the IWV. We use two different approaches: First, using the radiosondes in comparison to 20-min time averages from the model and HATPRO and second evaluating the entire time period using HATPRO and ICON-LEM.

As mentioned in Section 2.2, the IWV can be retrieved from the HATPRO as well as calculated from the radiosondes directly. At first, we look how well both the model and HATPRO compare to the radiosondes which we use as reference. For the calculation of the IWV from the radiosondes, we used the saturation vapor pressure formula derived by Goff and Gratch (1946). As the operationally launched radiosondes are only available once a day at 12:00 UTC, the IWV from HATPRO and the model were computed using a 20-min average from 11:00 to 11:20 UTC. In Figure 8, both (a) HATPRO and (b) ICON-LEM are plotted against the IWV from the radiosondes. One can see that the model has a larger spread but a smaller bias (-0.11 kg m^{-2}) than HATPRO (-0.41 kg m^{-2}). This bias becomes more visible in HATPRO for larger values as a linear regression (red line in Figure 8a) shows. This typical increase of uncertainties for larger values was also found by Nomokonova et al. (2019). What one can also see in Figure 8, is that there are fewer cases with higher values for the HATPRO selection. This is likely connected to the flagging applied for HATPRO and reveals an issue when exploring cases with high IWV. In such cases, precipitation is more likely which leads to a reduction of cases with high IWV in the observations and thus leads to a bias in the cases studied. This case reduction limits the generalization of the comparison between model and observations.

Figure 6. Histogram for the mean relative humidity between 500 and 600 m for all radiosondes from August to December 2020. The dashed yellow line marks the 87% value which is used as threshold to differentiate between radiosonde profiles which belong to the higher or the lower mode.

The time series of the IWV for the entire period (Figure 9) show that in general, the model captures the IWV very well with only a small bias of 0.19 kg m^{-2} and a root mean squared error of 1.14 kg m^{-2} when comparing ICON-LEM to HATPRO. It can be seen in Figure 9 that the IWV follows a prominent seasonal trend and decreases toward November and December, which is a typical feature to be expected for this location. Additionally, one can see that the shape of the frequency distributions of IWV (Figure 10a) match well. Both distributions have similar mean values (ICON-LEM 8.01 kg m^{-2}, HATPRO: 8.72 kg m^{-2}) as well as skewness (ICON-LEM: 0.9, HATPRO: 0.7). As mentioned in Section 2.2.1 there are uncertainties in the retrieval used for HATPRO. We experimented with taking the

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Figure 7. Drift trajectory for the radiosondes launched between August and December 2020 up to 1 km height. The blue set indicates drifts where the radiosondes have a mean relative humidity above 87% between 500 and 600 m, while the orange set includes drifts where the mean relative humidity is lower than 87%. (Topography source: Polar Institute Norway).

difference between HATPRO and the radiosondes into account by using the before mentioned linear regression (Figure 8a) to adjust the HATPRO measurements. Comparing these adjusted values to the simulations though, only showed minor differences in the anyways already good agreement between the model and the observations (Bias = -0.14 kg m^{-2} and RMSE = 0.94 kg m^{-2}).

Because water vapor is crucial for the development of clouds, we further investigated if there would be differences in the IWV histograms between the cloudy and clear columns (see methods in Section 2.2.2). This separation of columns yields a higher cloud occurrence in ICON-LEM (77%) in comparison to the observed cloud occurrence of 73% (Table 2). Both values though are in the range expected for an Arctic location and are sensitive

Figure 8. Integrated water vapor (IWV) for (a) Radiosonde versus Humidity And Temperature PROfiler (HATPRO) and (b) Radiosonde versus ICOsahedral Non-hydrostatic model (ICON) Large-Eddy model. For Humidity And Temperature PROfiler (HATPRO) and ICON, the IWV is taken as the 20-min average (11:00–11:20 UTC). Only days between August to December 2020 were used. Days where HATPRO was flagged, were excluded in (a) but not in (b). The least squares fit is shown by the red line defined by the given intercepts and coefficients. The identity line is marked by the blue dotted line.

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Figure 9. Integrated water vapor with time as measured by Humidity And Temperature PROfiler (turquoise) and simulated by ICOsahedral Non-hydrostatic model Large-Eddy model (red) between August and December 2020.

to the chosen thresholds to distinguish clear and cloudy cases. Interestingly, this differentiation between cloudy and clear columns does lead to larger inequalities in the IWV histograms although these too are not substantial (Figures 10b and 10c). Noticeable is the IWV range between approx. 13 and 20 kg m^{-2} in Figures 10b and 10c. In this range, ICON-LEM has more clouds and less clear sky than what is found in the observations. It is interesting that for these higher values HATPRO clearly shows clear sky cases exist (Figure 10c), but the cloud microphysics parameterization in ICON-LEM almost always produces clouds above IWV around 15 kg m^{-2}.

3.4. Liquid Water Path

The LWP is helpful to get an impression if the hydro- and thermodynamical processes in the model are able to convert the available water vapor into liquid water. It is not straightforward to retrieve vertical profiles of liquid water content resulting in high uncertainties (Ebell et al., 2010). Thus, we used Cloudnet to distinguish between clear versus cloudy columns (see Section 2.2.2). By using the LWP we evaluate if there is liquid in the cloudy columns. Based on that we distinguish between columns with liquid and mixed-phase clouds in contrast to columns which only contain ice clouds. The sensitivity of HATPRO leads to the necessity of setting a threshold for the LWP. We tried different LWP lower thresholds (5, 10, and 20 g m^{-2}) to determine how sensitive the results are to the threshold and used the accuracy of HATPRO as the highest threshold. In HATPRO the percentage of columns containing liquid ranged, depending on the threshold, from 70% to 53% (51,424–39,293 cases of total cloudy columns). This is a stark contrast to the 34%–26% (28,090–21,764 cases of total cloudy columns) of cloudy columns which contain liquid in ICON-LEM. Table 2 summarizes these numbers. One feature noticeable from these numbers is the average lack of liquid water in the model. On the other hand, this implies that too many pure ice clouds are produced in the model in contrast to what is observed. It appears that the model's

Figure 10. Histogram of percentage with overlaid smoothed distribution of integrated water vapor for (a) all columns, (b) cloudy columns, and (c) clear columns for ICOsahedral Non-hydrostatic model Large-Eddy model (red) and Humidity And Temperature PROfiler (turquoise). Histogram bin width 1.2 kg m^{-2}.

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Table 2
Cloudy Versus Clear Occurrence and Clouds Containing Liquid Based on Liquid Water Path Threshold, for ICOsahedral Non-Hydrostatic Model Large-Eddy Model and for the Observations (OBS, Combination of Humidity And Temperature PROfiler and Cloudnet)

			Clouds with LWP threshold g m^{-2}		
	Clear	Cloudy	LWP > 5	LWP > 10	LWP > 20
OBS %	27	73	70	63	53
ICON-LEM %	23	77	34	31	26

microphysical implementation favors the formation of ice particles when clouds develop. Similar findings have also been shown by (Nomokonova et al., 2019) for the same location using the ICON-NWP model with 13 km resolution and a one-moment microphysical scheme.

For the comparison of the LWP distributions, we selected only cases with LWP ≥ 10 g m^{-2} (Figure 11). Evaluating the remaining data showed that the LWP is more skewed toward higher values in ICON-LEM with a mean of 168 g m^{-2} whereas HATPRO shows no LWP larger than 1,171 g m^{-2} and has a mean of 91 g m^{-2}. Figure 11b makes it clear though that cases with high LWP (>400 g m^{-2}) are very rare also in ICON. The close-up using the linear scale (Figure 11b) shows that the distribution for the values below 400 g m^{-2} is similar. Looking at Figure 11a which uses a logarithmic scale a surprising extended tail of high LWP values in ICON-LEM becomes visible. These cases of high LWP are generally connected to precipitation but are not filtered out either because the precipitation does not reach the ground or because it occurs with a time shift. From these findings, the picture emerges that liquid-containing clouds seem to contain more LWP in the simulations than what is measured.

With the advantage of using this large data set covering many cases where there was no rain or drizzle, we can assume a certain reliability of the statistics. Combining the above-mentioned findings and the high accuracy of the IWV points toward shortcomings in the microphysical representation of production and growth of cloud droplets.

3.5. Simulated and Measured Precipitation

Continuing in the direction of droplet and ice crystal growth, the question arises of how well the precipitation is represented for this specific location. As mentioned in Section 2.2, one challenge for the precipitation measurements is to correct for the wind-induced undercatch, especially in the case of solid precipitation. A total of 368 hr with precipitation were observed between August and December 2020. We computed the Heidke skill score (HSS), based on the hourly resolved values, which gives an estimate of the quality of the precipitation occurrence prediction. With HSS = 0.43 we show that the hourly precipitation/no precipitation occurrence is well simulated. The false alarm rate, indicating when the model predicts precipitation but there is none, is quite low with 0.08 and a proportion correct of 0.87 signals that the time of precipitation/no precipitation is mostly met.

Another aspect regarding the precipitation is the intensity. To evaluate this the hourly accumulated precipitation is used. Figure 12 depicts the distribution of the hourly precipitation sums as simulated by ICON-LEM in

Figure 11. (a) Histogram of percentage of liquid water path (LWP) with overlaid smoothed distribution of LWP for ICOsahedral Non-hydrostatic model Large-Eddy model and Humidity And Temperature PROfiler for cases with LWP ≥ 10 g m^{-2}. The bin width is 50 g m^{-2} and the gray shaded area marks the values with increased uncertainties. (b) Zoom in of (a) for LWP values up to 500 g m^{-2} and linear *y*-axis. Histogram bin width is 25 g m^{-2}.

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Figure 12. Frequency distribution of hourly accumulated precipitation from August to December 2020. The olive bars show Pluvio with Wolff corrections (P-Wolff) and the red bars ICOsahedral Non-hydrostatic model Large-Eddy model (ICON-LEM). A limit of 0.05 mm hr^{-1} is set for the precipitation based on the limit of the Pluvio. The vertical lines at 1.75 and 2.03 mm indicate the 95% limit for ICON-LEM and P-Wolff, respectively.

comparison to the Pluvio observations using the Wolff correction (P-Wolff). From Figure 12 it is clear that the majority of the hourly accumulated precipitation is below 1 mm and few cases have more than 2 mm. Creating robust statistics for cases with higher values was therefore not possible with our limited data set. Nevertheless, the 95th percentile is slightly lower for ICON-LEM (1.75 mm) than for P-Wolff (2.03 mm). This points toward an underestimation in ICON-LEM of the precipitation amount for the more extreme precipitation cases during the analyzed period.

To gain an insight into the total amount of precipitation, the focus is now shifted toward the daily sums of precipitation. In Figure 13 the cumulative sum of the different accumulated daily precipitation classes are shown for the observations (original and corrected values) and the simulations. The spin-up time (00:00–03:00 UTC) is excluded in both sets. Further, the ICON-NWP values are included to highlight improvements gained from increasing the resolution. The total precipitation amount measured at the AWIPEV station for the analyzed time lies between 187 and 270 mm (olive and green lines in Figure 13). This range takes the different corrections into account and therefore gives an idea of the measurement uncertainty. If no corrections were applied, the total precipitation amount would lie at the lower limit of 187 mm (light green line). The corrections thus add here up to 44% to the originally measured precipitation amount. Days with accumulated precipitation higher than approx. 10 mm are the ones which the model is more likely to under represent. For instance the number of days with daily precipitation sums of more than 10 mm is 5 for ICON-LEM and just 1 for ICON-NWP in contrast to 7 for the observations (P-Wolff). Even though days with these larger precipitation amounts are also rare in the observations, they contribute to more than 50% to the total precipitation amount. So it is even more important for the models to capture these events. It is noticeable though that ICON-LEM (206 mm) improves the simulated amount in comparison to the ICON-NWP (107 mm) simulations significantly. What is important to keep in mind here is that they both use different microphysics schemes, one-moment for ICON-NWP versus two-moment in ICON-LEM. That ICON-LEM achieves a greater accuracy is somewhat expected behavior as local extremes are smoothed out more if the grid box decreases in horizontal resolution and relevant processes such as clouds are better resolved. Additionally, the microphysical processes and hydrometeors are represented in more detail in ICON-LEM.

Figure 13. Cumulative sum of daily accumulated precipitation for August to December 2020. The olive and green lines indicate the values measured with the Pluvio rain gauge without (P-No correction) or with correction (P-Forland, P-Wolff, and P-Kochendorfer). The model values are marked in red (ICOsahedral Non-hydrostatic model [ICON] Large-Eddy model) and blue (ICON-numerical weather prediction model). A limit of 0.05 mm hr^{-1} is set for the precipitation based on the limit of the Pluvio and bins of 2 mm day^{-1} are used. Data between 00:00 and 03:00 UTC is excluded due to the spin-up time.

4. Conclusions and Outlook

We presented the results of an extensive evaluation of ICON-LEM using a large data set of daily simulations. It covers 5 months from August to December 2020. These simulations were performed semi-operationally using a setup with lateral boundary conditions and heterogeneous surface types. It provided a remarkable basis for comparisons with different observational products. The motivation was to create a thorough and elaborate reference for those who apply this model in the Arctic. Further, we explored some limitations of our approach where we combine model data and observations and highlighted features special to Ny-Ålesund and its surroundings. Yet the results are not only relevant for the Arctic, but also from a general model development perspective, especially for the representation of clouds. The different aspects covered were (a) the representation of the wind, (b) humidity and temperature in the BL, (c) the IWV and LWP in the Ny-Ålesund columns, and (d) the precipitation. For the analysis, several instrument products from the AWIPEV super-site were used. These were an MWR, Cloudnet, a rain gauge, and radiosondes.

Starting with the wind, we found that the model captures the two different wind regimes in the BL and the free atmosphere very well. In the BL the higher resolution proves helpful leading to a more accurate distribution

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showing the channeling of the flow through the Kongsfjorden. The temperature profile is represented correctly but shows a cold bias for the model values especially toward the surface. The relative humidity comparison in the BL proved challenging as we found that the drifts of the radiosondes create a clear signal in the soundings. We, therefore, emphasize the need to consider the local variability in such a diverse surrounding. The bias increase toward the surface also motivates to consider aspects such as surface type representation.

Using the Cloudnet target classification we showed that ICON-LEM simulates around 4% more clouds than were observed. The cloud occurrence was in a typical range for Ny-Ålesund in both model and observations. The exact definition of what counts as a cloud depends on thresholds and sensitivities in the observations as well as the model, which may impact the cloud occurrence results. The similarities in the modeled and observed IWV were striking. The model can capture long and short term changes very well. An exception are clear sky cases with large IWV values which the model underestimates. Another interesting finding was the abundance of ice clouds in the model. Using the LWP (>5 g m^{-2}) we differentiated between columns containing liquid and those only containing ice. This distinction was then used to evaluate the occurrence of liquid water. In the observations up to 70% of the columns contained liquid whereas it was only up to 34% in the model. Further, in the LWP data from HATPRO no values are above 1,171 g m^{-2}. This limit is partially related to the fact that such high values are related to precipitation cases which are likely to be filtered out by the instrument's quality flag.

Combining the findings of IWV and LWP there are three limitations in ICON which are likely linked. (a) too efficient ice production, (b) overestimation of cloud occurrence, and (c) too much liquid water when droplets form. The linking factor is the cloud microphysical parameterization in the model. This does not only include how processes are implemented but also how the parameters are set. In first sensitivity studies we could see that switching to an alternative cloud condensation nuclei (CCN) scheme which included different numbers of CCN, showed different results in the hydrometeor composition. This will be part of further and more detailed research.

For the precipitation, we found a better agreement of ICON-LEM with the measured accumulated precipitation during that period than ICON-NWP. Both models underestimated the cases with daily high precipitation amounts. The ICON-LEM model shows a similar distribution for the hourly accumulated precipitation in comparison to the observations. However, ICON-LEM overestimates the frequency of occurrence of low amounts of hourly accumulated precipitation sums and underestimates the occurrence of very high amounts. During the evaluated period there were few cases with strong precipitation but these were important for the total precipitation amount.

This evaluation encourages the use of realistic high-resolution simulations to study changes in the Arctic related to Arctic amplification. Further, it enables us to focus on improving the cloud microphysical processes. Especially when it comes to the formation of cloud droplets and ice particles we saw that this can be improved. Additionally, it should be noted that the settings of this mountainous region and the strong contrasts in the surface composition highlight the adaptability of the model for complex terrain. Generally, the advantages of being able to perform realistic simulations for these challenging environments are not limited to the Arctic climate. In summary, this analysis shows the feasibility of running high resolution simulations for longer time periods, when focusing on a specified area of interest, and how we can benefit from the statistical analysis.

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Data Availability Statement

The observational data is available in PANGAEA. MWR HATPRO data: https://doi.pangaea.de/10.1594/PANGAEA.943004 (Ebell & Ritter, 2022). Radiosonde data: https://doi.org/10.1594/PANGAEA.914973 (Maturilli, 2020). The Pluvio and Cloudnet data is available on request. The meteograms of the simulations can be found in the data set "Ny-Aalesund ICON-LEM 600 m meteograms from August to December 2020" in the data catalog DOKU at DKRZ: https://www.wdc-climate.de/ui/entry?acronym=DKRZ_LTA_1086_ds00003 (Kiszler & Schemann, 2022). The ICON model code is available for institutions or individuals under a license: https://code.mpimet.mpg.de/projects/iconpublic/wiki/How%20to%20obtain%20the%20model%20code.

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6 IMPACTS OF AEROSOLS AND THEIR PARAMETERISATIONS ON CLOUD PROPERTIES

In Section 3.3, the formation of droplets and ice particles via activation and nucleation was discussed. A current challenge is that the impact of aerosols on cloud properties is partially unknown, and therefore, representing them appropriately in models is difficult (Burrows et al., 2022; Pierce and Adams, 2009). In Section 1.3, it was further discussed that the impact of aerosols on clouds is relevant to the Earth's energy budget. Therefore, this chapter explores how different INP and CCN parameterisations impact simulated clouds in the Arctic. To provide sufficient background on the parameterisation schemes, the first section will explain the activation and nucleation schemes which may be chosen in ICON. After that, the differences between these schemes and related studies are discussed. Then, simulations using different schemes are analysed and compared to explore the behaviour of the clouds. An observational data set is used as a reference to give an idea of whether one or the other parameterisation is better.

6.1 INP AND CCN SCHEMES IN ICON

The first CCN activation scheme which is presented is the CCN activation from Hande et al. (2016) (hereafter "Hande CCN"). This scheme was explicitly developed during the HD(CP)^2 project for use in ICON-LEM. The parameterisation combines several aerosols' chemical and physical properties while using a simple mathematical model to estimate the CCN concentrations. This model is a function of vertical velocity and atmospheric pressure (Figure 8) and indeed allows for a clear and comparably short implementation in the model code. In Figure 8, one can see that the amount of activated CCN increases with vertical velocity, which is argued to correspond to an increase in supersaturation. This connection is strongest for wind speeds between 0.1 and 2 m s^{-1} and is relevant when considering that the resolution of a simulation impacts the vertical velocity variation (Schemann, Ebell, et al., 2020). This vertical velocity variation can be quite low in the Arctic, where convection is not as strong (Shupe, Kollias, et al., 2008) as in warmer regions. Several aerosols from natural (sea salt, dust, organic carbon) and anthropogenic sources (ammonium sulfate, ammonium nitrate, elemental carbon, sulfate) were measured during the HOPE campaign (HD(CP)^2 Observational Prototype Experiment). These were used as the basis for the CCN activation parameterisa-

Figure 8: CCN activation spectrum as parameterised in Hande et al. (2016) and used in ICON. The CCN concentration dependency on the vertical velocity and the pressure is indicated by the different lines. Model data from their simulations using the aerosol parameterisation by Abdul-Razzak and Ghan (2000) is shown by the black dots, the fitted functions for each pressure level are the red lines. This figure from Hande et al., 2016 is published under the CC-BY 3.0 license by Copernicus Publications.

tion. In the context of the use of ICON in the Arctic, it is important to mention that Hande et al. (2016) found the anthropogenic fraction to be 80-90 %. This is more than the global average and not representative of an Arctic environment which is sparsely inhabited. Another aspect of the CCN distribution is that the concentrations are higher towards the surface (higher pressure levels) as more aerosols are emitted there. A downside of this simple approach is that it does not adapt to different aerosol concentrations and types and assumes all aerosol profiles follow the same functions at every time, i.e. no seasonality exists. Kretzschmar et al. (2020) tried to address this by using a modified and down-scaled version of the Hande CCN activation for a set of cases using ICON on a kilometre-scale. These changes showed improvements in the hydrometeor number concentration distribution. One of the proposed changes of the Hande CCN activation was adding a term to represent the subgrid-scale vertical wind distribution. This achieved better results for the cloud radiative effect in comparison to the standard parameterisation. As the reference was an Arctic airborne campaign (ACLOUD), they only had a very limited set of cases, though.

Another option which one can choose for the CCN activation is based on Segal and Khain (2006) (hereafter "SK"). This parameterisation can be implemented as a regression equation or using a look-up table. Same as for Hande CCN, the activation of CCN depends on the vertical velocity, but no height dependency, such as using the pres-

sure, is included in the regression equation and must be implemented independently. This height dependency was implemented in the past in ICON. Segal and Khain (2006) aimed at using this parameterisation in large-scale models, which cannot resolve the vertical velocity enough to produce the supersaturation required for the CCN activation. They use only sodium chloride ($NaCl$) as aerosol and assume that for any other aerosol, the " "effective" size distribution of $NaCl$ particles" can be calculated. Six different regimes are suggested to differentiate between locations with different CCN concentrations, the vertical velocity at cloud base (W_{cb}) and CCN size distributions, of which four are implemented in ICON (maritime, intermediate, continental, and "polluted" continental). Of the suggested regimes, the maritime stratus is characterised by "low [CCN] concentrations N_{cn}, wide [CCN] size distributions and small W_{cb}" and are chosen as more adequate for low-level Arctic clouds. In ICON, the parameterisation is implemented as an equidistant look-up table, and as in Hande CCN the activated CCN amount increases with vertical velocity.

Continuing with the colder regimes, ice nucleation comes into play. Here the nucleation schemes by Hande et al. (2015) and Phillips, DeMott, and Andronache (2008) are introduced (hereafter Hande INP and Phillips). The Phillips scheme includes three groups of aerosols, namely "dust/metallic, black carbon (here also referred to as soot), and insoluble organic aerosols". As INP concentrations, they use observations from a field campaign at higher elevations in Colorado and Florida to derive an empirical parameterisation. They evaluated the empirical parameterisation using laboratory experiments conducted in the AIDA cloud chamber. In ICON, three predefined settings are given where the amount of initial dust, soot and organic aerosols can be varied from high to low. The formation of ice depends on the saturation with respect to ice (S_i) as well as the temperature. Similarly, Hande INP uses the relative humidity, which can also be implemented as S_i, and temperature dependence of INP to create a best-fit function to estimate the INP number concentration. Hande et al. (2015) started with simulated concentrations of dust over Europe and used observational data to evaluate the results. They also differentiated between seasons, and these seasons are included in the ICON model. In ICON, one can choose between winter, spring (highest concentrations), summer and autumn. Both implementations include immersion and deposition nucleation but differ in temperature range. Phillips is implemented for the temperature range from -93 to -5 °C while Hande INP is active between -53 and -12 °C. Values below -53 °C are treated as if the temperature was -53 °C.

6.2 SELECTION OF INP AND CCN SCHEMES

The previous section described the different parameterisation choices for nucleation and activation in the Seifert and Beheng (2006) two-moment microphysics scheme in ICON. A short comparison of the parameterisations will help better understand the results in the following sections. There are some clear differences between the CCN activation schemes by Hande et al. (2016) and Segal and Khain (2006). The first aspect is that Hande CCN used several aerosol types to derive the regression function, including sea salt, which is believed to be a relevant CCN in the Arctic (Gong et al., 2023). SK, on the other hand, only used sodium chloride to derive their parameterisation. Additionally, Hande CCN includes a decrease of aerosols with pressure, while SK does not directly include a vertical component. In the ICON code, an exponential decrease of CCN number concentration, from 4 km on, was implemented in the past. Both use the dependence of activated CCN numbers on the vertical velocity. The largest difference, which is also the reason for the switch from the default Hande CCN to the SK scheme in the Arctic, is the choice of the aerosol number. Hande CCN is based on German aerosol concentrations, which are much higher than in the Arctic and include large anthropogenic emissions. Further, there is no option to choose predefined settings for other regions in Hande CCN, while this is possible in SK. As the description of the maritime case in SK matches the low-level Arctic clouds most from the given options, this one is chosen as the setting. Obviously, representing the variability of CCN concentrations is not possible in either scheme. It is worth noting that although this lies beyond the scope of this thesis, developing new Arctic INP and CCN parameterisations using recent observational data (e.g. Ullrich et al., 2017; Wex et al., 2019) would be necessary to improve the aerosol representation.

Continuing with the nucleation schemes, there too the variability of the INP typically observed in the Arctic cannot be represented, requiring further investigation into the plausibility of either scheme. As presented before, the Hande et al. (2015) nucleation scheme is derived from aerosol concentrations over Europe which leads again to the question of whether this is suitable in the Arctic. As no Arctic profile is yet available for INP in the Arctic in ICON, a switch to the Phillips, DeMott, and Andronache (2008) nucleation scheme is used with the lowest possible setting for aerosols (only initial dust). This scheme covers a large temperature range, including typical Arctic conditions of -70 - 0 °C, which could be advantageous, and is characterised by a reduced number of aerosols which is more fitting for the Arctic.

The relevance of a fitting aerosol scheme was demonstrated specifically for Arctic clouds in ICON in Mech et al. (2020) and Kretzschmar

et al. (2020). Mech et al. (2020) introduced the PAMTRA forward simulator with an example comparing two different ICON setups to radar data. One setup used a constant CCN and INP number, while the other used the CCN activation by Hande et al. (2016) and the nucleation by Phillips, DeMott, and Andronache (2008) in combination with prognostic CCN and INP. This led to significant improvements in the comparison of the radar reflectivities between the observations and the model for the cases they evaluated. The original simulations showed a strong underestimation of the radar reflectivity with a maximum of -20 dBZ, while the adapted version was much closer to the observed radar reflectivity with a maximum of +10dBZ. Kretzschmar et al. (2020) modified the Hande CCN scheme to better represent subgrid scale vertical velocity and scaled it to match the lower Arctic aerosol concentrations, showing significant changes and partial improvements in the hydrometeor size distributions for several Arctic cloud cases.

None of the adaptations made in the mentioned study have been evaluated for a large set of cases and while the changes by Kretzschmar et al. (2020) showed improvements in some aspects, other changes in the simulation output were not beneficial. Thus the decision was made to apply similar changes as in Mech et al. (2020) and to evaluate this for a larger set of cases. In summary, the changes used in this thesis are the following: The default version uses a combination of Hande CCN & Hande INP (denoted as "Hande"), which was changed to SK CCN & Phillips INP (denoted as "SK-P"). Technically speaking, the combined switch of CCN activation and INP nucleation scheme is a change in the code from
`cloud_type_default_gscp4 = 2103, ccn_type_gscp4 = 1` to
`cloud_type_default_gscp4 = 2803, ccn_type_gscp4 = 6`. This chapter will give an overview of the changes due to the adapted INP and CCN settings. Specifically, the cloud occurrence, phase-partitioning and integrated humidity variables are investigated. The adapted ICON setup is subsequently used in the following Chapter 7 to evaluate the microphysical processes in Arctic low-level clouds.

6.3 COMPARISON OF DIFFERENT AEROSOL CHOICES

6.3.1 *Meteorological conditions during the evaluated period*

To compare the cloud microphysical compositions and the cloud occurrence, the simulation data of August and October 2021 is used. These months were chosen as the temperature and moisture levels capture two different regimes. In August and the beginning of October, 01.-30.08. and 01.-04.10. (period 1, P1), the IWV ranged from 10

to over 20 kg m^{-2} and decreased abruptly between 05.10. and 09.10. after which it remained between 2.4 and 9 kg m^{-2} (period 2, P2). P1 and P2 are visible in the IWV distribution (Figure 9 a), where the first mode represents the dryer P2 and the second mode the moister P1. Rain was common during P1, while snow and graupel only seldom appeared during that time but were the dominant form of precipitation from 6.10. on. Also, in the temperature, the two periods are visible. The lowest model level (≈20 m) temperature was above freezing in P1, where the temperature ranged from 0 to 9 °C. After 6.10. the temperature decreased from around 2 °C to minus degrees with a minimum of around -14 °C on 20.10.. This change of regimes allowed for MPCs with higher liquid amounts in August and the beginning of October (P1). The number of MPCs decreased towards the end of October, providing clouds with different phase-partitioning for the analysis. As thermodynamic variables such as temperature, wind, and pressure show no large differences between the two ICON setups overall, the focus of the next sections lies on cloud variables.

6.3.2 *Cloud occurrence and phase-partitioning*

Before looking more into the details of the clouds, it is worth spending a moment evaluating the integrated values. The advantage with integrated values is that accurate observations for the LWP and IWV exist in Ny-Ålesund (microwave radiometer HATPRO, see Section 4.1), which enables a comparison of simulations and measurements. In Figure 9, the IWV, LWP, IWP are illustrated for the simulations and the observations using HATPRO. As HATPRO does not provide consistent measurements when there is rain, cases with rain (>0.05 kg m^{-2}) are also excluded from the simulation data. If one does not exclude the cases with rain, the IWV distribution is almost identical for both setups, and both overestimate the mean IWV (Hande: 10.18 kg m^{-2}, SK-P: 10.17 kg m^{-2}, HATPRO: 9.20 kg m^{-2}). Excluding the rain cases (Figure 9 a), it can be seen that SK-P has slightly lower IWV values than Hande which also shows in the mean values (Hande: 8.31 kg m^{-2}, SK-P: 7.19 kg m^{-2}). The IWP only shows slight differences between both simulations (Figure 9 c) with Hande having a mean value of 14 g m^{-2} and SK-P 12 g m^{-2}. The LWP is definitely the variable with the largest difference between the simulations. Two features are relevant in Figure 9 b. One is that SK-P better captures the LWP values below 400 g m^{-2} while Hande can also simulate higher observed LWP values. The second feature is that the majority of cases are below 500 g m^{-2} making it more relevant to capture these values accurately.

Continuing with the cloud occurrence, Table 1 shows that the total cloud occurrence is higher for Hande (77 %) in comparison to SK-P (72 %). This can be further split into low, middle and high clouds,

which can occur simultaneously. The decrease of total cloud occurrence in SK-P is mainly attributed to a change in middle and high cloud occurrence by 3 and 11 %, respectively (Table 1). Interestingly, the low-level clouds (LLC) only decreased by 1 % for SK-P.

Another intriguing aspect in light of the lack of liquid-containing clouds in ICON-LEM found in the previous study (Kiszler, Ebell, and Schemann, 2023) is the question of whether the phase-partitioning is influenced by the change of CCN and INP activation. To further distinguish the cloud types, the clouds (including precipitation) are separated into pure ice, pure liquid and mixed-phase (Table 1). The threshold for the mass mixing ratio is 10^{-8} kg kg^{-1}. Further, only cases with temperatures above -40 °C were used as no liquid is available below that and therefore, no change in phase-partitioning, no matter which parameterisation is chosen, was found. It was found that the liquid cloud occurrence decreases from 21 % in Hande to 15 % in SK-P (-5 %). These clouds also seem to be thinner in SK-P than in Hande if one considers the distribution of the LWP, which shows lower values for SK-P (Figure 9 b). Additionally, the number of pure ice clouds increased by 5 % from 72 to 77 % for SK-P, while as discussed before, the IWP distribution remains similar in both versions (Figure 9 c). The mixed-phase clouds showed only a slight change of less than 1 %.

Digging deeper into the mixed-phase clouds, only clouds containing ice and droplets simultaneously are considered. Noticeably, the choice of activation and nucleation scheme does not impact the temperature range at which MPC occur (Figure 10, dashed lines). Both ICON-LEM setups have almost no MPC below -20 °C. The distribution of the supercooled liquid fraction (SLF) can further give insights into the composition of MPC. Based on Komurcu et al. (2014), the SLF is calculated using the mixing ratios of cloud droplets ($r_{\text{liquid water}}$) and cloud ice (r_{ice}) as

$$SLF = \frac{r_{\text{liquid water}}}{r_{\text{liquid water}} + r_{\text{ice}}}.$$

A SLF of 1 means the cloud is purely liquid, and 0 it is purely frozen. It can be seen that for SK-P, the mean SLF lies between 0.96 and 0.85 above -18 °C. Below -18 °C, most clouds in the simulated period are glaciated. Therefore, no reliable statement for lower temperatures can be made. For Hande, the mean SLF starts around 0.96 and begins to decrease below -7 °C until it is around 0.75 at -18 °C. The mean SLF values agree with the results in Shaw et al. (2022) derived from the simulations with the CAM model and satellite observations (CALIOP). While SK-P has an SLF which is closer to the cloud top values which Shaw et al. (2022) found, Hande is closer to the cloud-

	TOTAL	LOW	MIDDLE	HIGH	LIQUID	MIXED	ICE
SK-P (%)	72	54	57	37	15	8	77
HANDE (%)	77	55	60	48	21	7	72

Table 1: Cloud occurrence (%) and cloud phases (%) for simulated clouds in Hande and SK-P in August and October 2021 simulations. The cloud phase is only given for cases where the temperature is above -40 °C.

Figure 9: Integrated values for Hande (simulation data, blue) and SK-P (simulation data, red), and the HATPRO IWV and LWP (observation data, orange) for August and October 2021. a) Integrated water vapour (IWV), b) Liquid water path (cloud droplets, LWP), and c) Ice water path (cloud ice, IWP). A threshold of 0.01 kg m^{-2} is used for the LWP. The inlay figure in b) zooms into the LWP range from 0 to 0.4 kg m^{-2}. Cases with rain are excluded from the ICON data to mimic the flags applied in HATPRO.

bulk values.

6.3.3 *Hydrometeor composition*

The hydrometeor composition is also of interest as changes to the number of INP and CCN will cause changes in the total number of each hydrometeor type. What is very clear is that the SK-P version has fewer activated CCN and, as a consequence, fewer cloud droplets in parts two orders of magnitude (Figure 11 a). Fewer CCN further leads to a lower cloud droplet mass mixing ratio, illustrated in Figure 11 f. As a consequence of the low droplet number, it is possible that the droplets can grow more, as more vapour is available for a single droplet. This explains the increase in the raindrop number and a shift of the mass towards higher values (Figure 11 d and i). Interestingly, the difference is not so clear for the cloud ice, although there are slightly higher number concentrations for SK-P (Figure 11 b and g). The number of snow particles and amount of snow mass is almost

Figure 10: Mean supercooled liquid fraction (SLF) and number of cases which are mixed-phase for temperature bins (1 K intervals). Blue shows the Hande data, and red shows the SK-P data. Solid lines are for the SLF and dashed for the number of mixed-phase cases.

identical (Figure 11 c and h) for both setups, while the graupel mass and number concentration increases strongly in PK-S (Figure 11 e and j). This seems counterintuitive as the number of cloud droplets is actually less for SK-P, so one might think less riming would occur, causing less graupel production, but the opposite seems to be the case. The number of ice particles possibly matters more in this context, as even though the droplet number decreases strongly, they are still abundant. A possible step further would be to analyse the process rates for different INP and CCN settings to see if this hypothesis is true. Another feature that is noticeable in the number distributions is that they are strongly skewed towards high numbers.

The skewness of the number and mass distributions makes the mean value less informative if one looks at vertical and temperature profiles. Therefore, additionally, the median and the interquartile ranges (IQR) are used, as shown in Figure 12 and Figure 13, to evaluate the temperature distribution. The temperature distribution is similar to the vertical distribution. Therefore, only the temperature is shown here and the vertical distributions can be found in the Appendix Section A.2. For the mass mixing ratios and number concentrations, it can be seen that the snow and cloud ice profiles are very similar throughout most of the temperature ranges (Figure 12 d,e and Figure 13 d,e). Hande shows higher cloud ice concentrations below ca. -40 °C and below -50 °C (above ca. 6 km) also, the mixing ratio is higher. The vertical distribution (Figure 15) indicates that towards the ground, the ice mass in Hande decreases and is less than in SK-P. While the snow number concentrations and mixing ratios are strikingly similar in both versions' vertical and temperature distributions, slight differences appear below ca. 3 km. There Hande shows slightly

Figure 11: Distributions of number concentrations (left column) and mass mixing ratios (right column) for August and October 2021 for different hydrometeor types and simulations versions. Blue colours indicate results from the Hande simulations, and red is the SK-P simulations. The number concentration x-axis and the bin sizes are chosen to fit the hydrometeor type shown and differ between a) to e).

higher mass mixing ratios, corresponding to the temperatures between -10 °C and slight plus degrees. More considerable differences can be found for other hydrometeors. The cloud droplets follow similar profiles, although there is a constant offset between SK-P and Hande, where SK-P is lower (Figure 12 a and Figure 13 a). These differences are expected due to the lower CCN number in SK-P and they seem to increase towards higher temperatures for the cloud droplet concentration. Possibly as a consequence of the lower cloud droplet number, the amount of rain is much higher with a larger spread in SK-P, visible both in mass and in number concentrations (Figure 12 b and Figure 13 b). While the mass mixing ratio for SK-P shows an apparent decrease with decreasing temperature, the maximum of the raindrop number concentration lies between -5 and 0 °C, depending on the statistical measure used. The substantial increase of graupel in SK-P interestingly lies in the same temperature range as the largest rain increase (Figure 12 c and Figure 13 c) suggesting a link between both, possible microphysical processes linking rain and graupel being riming or rain freezing. In Figure 13 f, one can see that the number of activated ice nuclei is much higher in Hande than in SK-P. The majority of the activated ice nuclei can be found in regions below -40 °C (approx. above 6 km). Therefore, the higher number of available INPs in Hande can explain the higher amount of high clouds for Hande, which was mentioned before. The limitation of INP activation to relatively high clouds indicates that the CCN setting may be more important than the INP setting for the representation of mixed-phase clouds, which are typically low clouds. Further, the amount of snow and ice seems not to be strongly affected by the nucleation scheme change.

6.4 DISCUSSION AND CONCLUSIONS

As simulated clouds are sensitive to the CCN activation and INP nucleation schemes, different ones were explored in this study. The choice was made to use the default scheme for this ICON setup in one simulation set and a scheme that more closely matches the Arctic reality in a second simulation set. The default INP and CCN schemes (Hande et al., 2015, 2016) were compared against the maritime INP and CCN schemes (Phillips, DeMott, and Andronache, 2008; Segal and Khain, 2006). The direct comparison of two months of simulations with both setups showed major changes impacting the LWP, hydrometeor composition, cloud occurrence, and cloud phase. The amount of cloud droplets was drastically lower in SK-P than in Hande, which was to be expected for the lower CCN activation numbers. This further affected the raindrops, which were more numerous in SK-P. Additionally, the graupel mass and number concentration were larger for SK-P. In contrast, the ice and snow particles were only

Figure 12: Temperature distribution of the hydrometeor mass mixing ratios in August and October 2021 for cloud droplets (a), rain (b), graupel (c), snow (d), and cloud ice (e). Note that the scaling of the x-axis in a) differs from the rest. The dashed lines show the median, the solid lines the mean, and the interquartile ranges (IQR) are marked by the shaded areas. Blue colours are for the Hande simulations, and red is for the SK-P simulation.

Figure 13: Temperature distribution of the hydrometeor number concentrations in August and October 2021 for cloud droplets (a), rain (b), graupel (c), snow (d), cloud ice (e) and the number of activated ice nuclei (f). Note the logarithmic x-axis in a). The dashed lines show the median, the solid lines the mean, and the interquartile ranges (IQR) are marked by the shaded areas. Blue colours are for the Hande simulations, and red is for the SK-P simulation.

slightly affected by the change except when it came to very cold temperatures, where the higher number of INP in Hande became very visible.

In total, the cloud occurrence increased with increasing CCN and INP concentrations which matches studies such as Mauritsen et al. (2011). Albrecht (1989) proposed that the cloud fraction of shallow marine clouds decreases with low CCN concentrations due to the faster formation of precipitation, which shortens the cloud lifetime. In this study, the decrease of LLC occurrence with decreasing CCN was not so clear, though. The change of only 1 % in LLC occurrence with lower numbers of activated CCN does not clearly support the hypothesis that if aerosols are less abundant, the hydrometeors will grow more and therefore precipitate more, decreasing the cloud lifetime. The number and mass of rain did increase drastically for SK-P where the CCN number is lower, something also seen in Barrett and Hoose (2023) for decreasing CCN numbers, but the clouds still maintained themselves in many cases. This means that other factors also seem to play a significant role and that the model might not be able to capture this feature correctly in comparison to observations. The difference of the high cloud occurrence, which was 11 % more for Hande, can be explained by the large difference in INP amount for higher cloud layers (shown in Figure 13), connected to lower temperatures.

Another expectation was differences in the phase-partitioning of clouds between both parameterisation choices. This was indeed the case as ice clouds became more frequent, and the amount of liquid clouds reduced in SK-P. The change of settings only had a limited effect on the occurrence of mixed-phase clouds though. In comparison to previous observations of MPCs in Svalbard, the occurrence frequency seems rather too low for both settings (Gierens et al., 2020; Mioche et al., 2015; Nomokonova et al., 2019). Future research using remote sensing data could shed more light on this. The supercooled liquid fraction was used to further evaluate the phase-partitioning in MPCs. Here it could be seen that, on average, SK-P had higher values and did not show such a clear decrease with temperature as Hande did. Further, the percentage of MPC was almost the same for both versions. This, combined, suggests that the INP and CCN impact the phase-partitioning, but other factors may determine whether a MPC will persist or, for instance, glaciate fully. Komurcu et al. (2014) also found that changing the ice nucleation parameterisation did not decrease the spread in the cloud phase-partitioning of the GCMs which they studied. It is possible that glaciation may be occurring faster in the SK-P simulations, and fewer clouds can exist in the intermediate phase state, which causes the mean SLF to be larger than 0.85 above

-18 °C.

Choosing suitable location-dependent INP and CCN parameterisations is an important step in simulating clouds correctly. In comparison to the observations, neither setup was able to capture the full distribution of the LWP accurately. But an important aspect is that in the regime of LWP $< 500\,\mathrm{g\ m^{-2}}$, SK-P did show improvements to the LWP. This is crucial because very few cases have higher LWP values, and motivates our choice to continue with the SK-P simulation setup. Conversely, it is questionable if the strong increase in rain for SK-P is fitting. These findings imply that improvements to the current nucleation and CCN activation schemes and, potentially, the microphysical processes are necessary. Accurate CCN and INP parameterisations can also show us where there are possibly compensating errors, as many parts of the model have been tuned to achieve the best results. The tuning makes sense for weather predictions, but the phase-partitioning is crucial for climate predictions, where the radiation budget must be right. Further research is needed into this topic, and implementing a thoroughly tested Arctic aerosol profile, for example, with the use of observational data such as presented in Wex et al. (2019), would be a good step to take in ICON. Another factor that was mentioned was the implementation of microphysical processes. In the end, these determine what will happen after the nucleation/activation and how the hydrometeors interact. One can see that the CCN and INP are not the only factors influencing the phase of a cloud. Therefore, the next study addresses the question of which processes determine the phase-partitioning and provides a look into the regimes in which they are active in.

7

MICROPHYSICAL PROCESSES IN LOW-LEVEL ARCTIC CLOUDS

The last study focuses on the third research question regarding the influence of microphysical processes on the phase-partitioning of Arctic low-level clouds. It is a pure model study as these processes cannot be observed in the field. As one could see in the previous study, changing the aerosols strongly impacts the cloud's composition, but the number of mixed-phase clouds remained almost the same. This indicates that the microphysical processes potentially have more influence than the aerosols alone on creating and depleting mixed-phase regimes. Therefore, the aim is to provide a better understanding of which microphysical processes are the dominating phase changers. The manuscript has been submitted and is presented here in that state.

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Microphysical processes involving the vapour phase dominate in simulated low-level Arctic clouds

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Abstract. Current general circulation models struggle to capture the phase-partitioning of clouds accurately, either overestimating or underestimating the supercooled liquid substantially. This impacts the radiative properties of clouds. Therefore, it is of interest to understand which processes determine the phase-partitioning. In this study, microphysical process rates are analyzed to study what role each phase-changing process plays in low-level Arctic clouds. Several months of cloud-resolving ICON simulations using a two-moment cloud microphysics scheme, are evaluated. The microphysical process rates are extracted using a diagnostic tool introduced here, which runs only the microphysical parameterisation using previously simulated days. It was found that the importance of a process varies for the polar night and polar day, although phase changes that involve the vapour phase dominate. Additionally, the dependence of each process on the temperature, vertical wind and saturation was evaluated. Going a step further, we used the combined evaporation and deposition rates to demonstrate the Wegener-Bergeron-Findeisen process occurrence. This study helps to better understand how microphysical processes act in different regimes. It additionally shows which processes play an important role and contribute to the phase-partitioning in low-level Arctic clouds. Therefore, these processes can be better targeted for improvements in the model that aim to better represent the phase-partitioning of Arctic low-level mixed-phase clouds.

1 Introduction

Several studies (Ebell et al., 2020; Shupe and Intrieri, 2004; Curry and Ebert, 1992) showed the importance of clouds for the Arctic radiative budget. Clouds further play a role in different feedback mechanisms, for instance, the cloud-phase feedback (Mitchell et al., 1989), and either amplify (positive feedback) or dampen (negative feedback) the warming. As the Arctic is warming up to four times faster than the global average (Rantanen et al., 2022), it is of interest to which extent clouds play a role. Currently, the question still remains though whether the total cloud feedback is positive or negative (Middlemas et al., 2020; Goosse et al., 2018). A specific challenge is the cloud-phase feedback as the changes in the cloud's phase-partitioning impact the cloud radiative effect (Mitchell et al., 1989; Storelvmo et al., 2015). The reason for these uncertainties regarding the cloud feedbacks stems from the difficulties of models on all scales to represent clouds, especially mixed-phase clouds (MPCs) accurately (Kay et al., 2016; Zelinka et al., 2020). These difficulties are connected to the complexity of microphysical processes in clouds and their parameterisations in models. One consequence is that many models are unable to capture the

phase-partitioning in clouds correctly (Tan et al., 2016). As a result, it is hard to quantify cloud feedbacks causing uncertainties in the climate projections (Zelinka et al., 2020).

Some models struggle to represent supercooled liquid in MPCs and often underestimate it (Cesana and Chepfer, 2012; Kiszler et al., 2023). Huang et al. (2021) link this underestimation of cloud liquid in the CESM1 model to the Wegener-Bergeron-Findeisen (WBF) process, where ice grows at the expense of liquid water due to the lower saturation required above frozen surfaces. While sometimes the limited spatial and temporal resolution can cause the full glaciation of a cloud (Storelvmo and Tan, 2015), other studies showed the importance of the WBF process to estimate the climate forcing of MPC correctly (Shaw et al., 2022; McGraw et al., 2023). In contrast, Zhang et al. (2020) found an overestimation of liquid in the E3SM model after several changes, including a switch in the ice nucleation scheme (new: Classical Nucleation Theory, Wang et al., 2014) and microphysical parameterisation scheme (new: Gettelman and Morrison, 2015). Again, this shows that the phase-partitioning and representation of cloud microphysical processes remains a challenge (Korolev et al., 2017; Morrison et al., 2020).

To understand where these uncertainties come from and address them, many studies have used sensitivity tests by varying process parameters or aerosol concentrations, where the subsequent changes of the cloud macro- and microphysics and other model components are evaluated (e.g. Lasher-Trapp et al., 2018; Shaw et al., 2022). This can provide valuable insights but makes it hard to untangle the exact contribution of each process. Additionally, the number of feasible model runs cannot cover the full range of possible parameter changes and combinations. Another approach aims to evaluate the microphysical process rates directly. This was done, for instance, by Gettelman et al. (2013) for a general circulation model (GCM) to look at the relative importance of microphysical processes in climate models using daily rates. In a recent paper, Barrett and Hoose (2023) used so-called microphysical pathways, which include different sets of microphysical processes, to study an idealized deep convective system. Kalesse et al. (2016) found a strong connection between the deposition rate of snow and the snow mass mixing ratio in a case study of an Arctic low-level cloud. Fan et al. (2017) studied the effect of changing ice nucleating particles (INP) and cloud condensation nuclei (CCN) concentrations on process rates, finding an increase in condensation, evaporation, deposition, sublimation and riming with increasing aerosols.

This study uses microphysical process rates to determine which processes contribute most to phase changes in Arctic low-level clouds (LLC). The focus lies on Svalbard, where LLCs frequently occur (Gierens et al., 2020; Nomokonova et al., 2019). Svalbard has an above average occurrence of MPCs (45-60 %) in comparison to the rest of the Arctic (30-50 %, Mioche et al., 2015) making the location ideal for studying the phase-partitioning of clouds. Cloud-resolving simulations with ICON-LEM are used to explore the importance of the microphysical processes for the phase-partitioning. To achieve this, a diagnostic tool is introduced, which provides the process rates using the simulation output as input. Several aspects are taken into account in the evaluation, those are the difference between polar night and day, temperature, vertical wind and saturation regimes. Additionally, we use the deposition and evaporation rates to evaluate if and how the WBF process impacts the amount of liquid and frozen hydrometeors in the simulated clouds.

2 Methods and data

2.1 Model simulations and data selection

The ICON-LEM (Dipankar et al., 2015; Heinze et al., 2017) simulations which we performed cover a circular domain with approx. 100 km diameter centred in Ny-Ålesund (Svalbard, lon-lat) and run with approx. 600 m resolution. The general setup follows the papers by Kiszler et al. (2023) and Schemann and Ebell (2020) with each simulation covering 24 h, although the first 3 hours are excluded in the analysis to avoid the spin-up. The forcing is from a 2.4 km ICON-NWP simulation, which is run on a larger domain and forced by the German weather service global ICON-NWP runs. The turbulence is parameterised by a 3D-Smagorinsky scheme (Dipankar et al., 2015). The two-moment scheme from Seifert and Beheng (2006) with an added hail class Blahak (2008) is used for the microphysics (referred to as SB). A slight adaptation was made to the default ICON microphysical settings. We use the Segal and Khain (2006) cloud condensation nuclei (CCN) activation with maritime aerosols, as well as the heterogeneous ice nucleation from Phillips et al. (2008) with the maritime aerosol concentrations. The output is given in the form of the vertical column above the grid cell containing Ny-Ålesund (meteogram) for every 9 s on 150 levels. This output includes the following hydrometeor mass mixing ratios and number concentrations: cloud droplets, rain, ice, snow, graupel and hail.

For the analysis, a subset of the data, which only includes low-level clouds, was created. This was done by first selecting all grid boxes which are cloudy using a threshold for the hydrometeor concentration of 10^{-8} kg kg^{-1} (same as in Kiszler et al., 2023; Schemann and Ebell, 2020) above which a grid box is defined as cloudy. For a cloud to be classified as low-level, the cloud top height must be below 2.5 km (same as Gierens et al., 2020; Chellini et al., 2022). Additionally, precipitating hydrometeors are not differentiated from non-precipitating ones. Therefore, a cloud with rain, graupel, hail or snow that reaches the ground will have a cloud base height at the ground. Further, if there is a cloud with a cloud top height higher than 2.5 km above the low cloud, we only use these cases if the higher cloud's bottom height is at least 500 m higher than the low cloud's top height. The frozen and liquid hydrometeors are grouped in the analysis to focus on phase transitions. The frozen mass mixing ratios ("frozen mass", kg kg^{-1}) is the sum of cloud ice, graupel, hail, and snow, and the liquid mass mixing ratios ("liquid mass", kg kg^{-1}) is the sum of cloud droplets and rain. The occurrence of low-level clouds and their composition varies between seasons (Mioche et al., 2015). Therefore, two sets of data are used. One covers the polar night (November 2021 - February 2022) and one the polar day (May-August 2021). In total, for the polar night, there are around 26.3 days' worth of low-level clouds, and for the polar day, there are around 37.9 days.

2.2 Microphysics parameterisation wrapper

To extract the process rates, this study uses a "microphysical parameterisation wrapper". The goal is to provide a simple diagnostic tool with spatial and temporal flexibility. Therefore, we chose to run the two-moment SB scheme and the saturation adjustment (for condensation/evaporation) independently from the model. A meteogram (single column) or 3D output file from

a previous simulation can be used as input for the wrapper. The model output is provided as input to the microphysical scheme in each timestep. It computes a single timestep, writes out the rates and continues with the following timestep. This approach allows the use of previous simulations from which the meteogram or 3D output of the required variables exists.

This approach has the clear advantage of being very fast compared to rerunning a full simulation, and one can focus on single processes. Further, outputting an entire domain of microphysical process rates is extremely space-consuming in most cases and can be avoided by just using a spatial and/or temporal selection. Another advantage is that the values of the thermodynamic variables (temperature T, pressure p, vertical velocity w, density ρ) are known exactly when they are used to compute the processes. This is not the case if one runs the entire model and outputs the thermodynamic variables only after additional physics and dynamical schemes have run. Additionally, it is possible to explore potential sensitivities of microphysical processes by applying changes inside of the wrapper and using it as a test suite. As this tool is simplified and only captures a part of the model, the advantages come with some limitations. One must keep in mind that any transportation (advection and precipitation) of hydrometeors cannot be included as the model itself is not run. In this study, we are only interested in the microphysical processes. Therefore, this is not an issue.

The mass change due to a process is computed by taking the difference between the mass before and after the process and is called (ΔQ_{proc}). Here, a timestep (Δt) of 3 seconds is used for the time integration. Therefore, the process rate ($\frac{\Delta Q_{proc}}{\Delta t}$) is given as the hydrometeor mass mixing ratio change over 3 seconds and is denoted as the "tendency" (kg kg^{-1} 3s^{-1}) in the following sections. As mentioned before, the hydrometeors are summed up into a liquid and frozen mass. The same is done with the processes, meaning, for example, that deposition is the sum of deposition onto ice particles, snow, graupel and hail. In this study, only processes that cause phase changes are included, as we are interested in processes that contribute to the phase-partitioning. E.g. frozen collisions are not evaluated as all frozen hydrometeors are summed up to a single class and compensate each other. Many of the processes evaluated in this study have self-explanatory names. Nevertheless, a brief process summary is given here and in Table 1 to prevent misunderstandings.

Deposition and Sublimation includes either the decrease or increase of water vapour due to phase changes from frozen to vapour. They are computed by the same process and split into negative (sublimation) and positive (deposition) contributions to the frozen mass.

Homogeneous and heterogeneous ice nucleation describes as one part the homogeneous nucleation of liquid aerosols, although it is rarely cold enough (T<30 °C) in the clouds used in this study to happen. The heterogeneous nucleation describes nucleation via immersion freezing and deposition nucleation. The parameterisation follows as mentioned Phillips et al. (2008). As homogeneous cloud droplet freezing did not occur for the low-level clouds, it is neglected here.

CCN activation describes the activation of cloud condensation nuclei following the parameterisation of Segal and Khain (2006).

Frozen evaporation and Melting refer to the melting of frozen hydrometeors, which can entail evaporation, but both are treated separately, leading to a process called "evaporation" also for the frozen hydrometeors.

Riming describes the accumulation of liquid mass on a frozen hydrometeor by decreasing the liquid mass and increasing the

Process	ΔQ_L	ΔQ_F	ΔQ_v
Ice nucleation	-	+	-
CCN activation	+	/	-
Deposition	/	+	-
Sublimation	/	-	+
Evaporation	-	/	+
Condensation	+	/	-
Riming	-	+	/
Rain freezing	-	+	/
Melting	+	-	/

Table 1. Impact of each process on the hydrometeor masses for liquid (ΔQ_L) and frozen (ΔQ_F) as well as the water vapour (ΔQ_v). The liquid class contains cloud droplets and raindrops, the frozen class contains ice particles, snow, graupel, and hail. A plus indicates an increase in the hydrometeor mass, and a minus a decrease.

frozen mass. In SB in ICON, this also includes the Hallet-Mossop secondary ice production, and if T>0 °C enhanced melting after riming will take place, making the frozen mass increase due to riming smaller.

Condensation and Evaporation includes either the decrease or increase of water vapour due to phase changes from cloud droplets and raindrops to vapour. They are the positive (condensation) and negative (evaporation) contributions of the saturation adjustment to the liquid mass.

Rain freezing only includes the freezing of raindrops and not cloud droplets. As both are summed up, though, this causes a decrease of the total liquid mass while the total frozen mass increases.

3 Results

3.1 Dominating processes in low-level clouds

We used a simple but straightforward approach to understand which processes dominate the phase-partitioning in low-level clouds. For each process, the mean value over all cases was computed. The mean values can vary, for instance, with temperature, as shown in the next section, so the percentage of occurrence, where a process makes up for over 1 % of the total mass change, is used as a second metric. The outcome of this is shown for all processes in Fig. 1 split into polar night (a) and polar day (b). The further a process is towards the upper right corner, the more relevant it is considered to be. One can see that there are some differences between the same processes for liquid and frozen hydrometeors. That is partially because some processes affect liquid, frozen and vapour at the same time, so the mean does not overlap in all cases. Additionally, there is numerical noise, which is why a minimum threshold for the tendency of $\frac{\Delta Q_{proc}}{\Delta t} > 10^{-18}$ kg kg^{-1} 3s^{-1} is set. As mentioned earlier, only

processes which contribute to phase changes are included here.

What becomes very clear from Fig. 1 a) and b) is that sublimation, deposition, and evaporation happen very frequently and also have the highest mean values. During the polar day (Fig. 1 b) it is visible that while evaporation and deposition still play a large role, sublimation has become less frequent. However, there is much less ice in general during the polar day, and most simulated clouds were purely liquid during that time. Melting, evaporation due to melting, and rain freezing all show mean tendencies above 10^{-12} kg kg^{-1} but occur below 20 % of the time, although the differences between the seasons are striking. During the polar day, rain freezing and melting increase in importance, possibly due to the difference in temperature regimes, which allows more precipitation to melt or more liquid precipitation to occur, which can then freeze. Ice and liquid sources via nucleation tend to occur quite seldom, as one can see from the CCN activation (CCN act., in Fig. 1) and the homogeneous & heterogeneous nucleation (Hom. & Het. nuc. in Fig. 1). Using the mass change as a metric for nucleation can be misleading as the number of hydrometeors produced can say more about the impact of the nucleation process than the mass change. Another finding is the imbalance between condensation and evaporation. This indicates that evaporation, acting as a sink of liquid, is stronger than the source of liquid via condensation. This is likely a local feature as only the single column of Ny-Ålesund is used here. This feature indicates that the microphysical processes may also have a strong location dependency. For instance, in Ny-Ålesund, the air over the fjord is more moist than over the land (Kiszler et al., 2023), which may cause more evaporation over land if a cloud is advected there. Nevertheless, the message in Fig. 1 is clear that the phase changes between liquid and vapour, as well as frozen and vapour, dominate, while processes contributing to phase changes between liquid and frozen are not as relevant.

3.2 Regimes of phases

To get an overview of the cases used for the second part of the analysis, it is beneficial to understand which temperature (T), vertical velocity (w), and ice/water saturation (S_i/S_w) regimes exist for the occurrence of the hydrometeors. These variables were chosen as the microphysical processes are directly connected to them. For the analysis, we will exclusively consider grid points identified as cloudy.

An overview of the distributions of the T, w and S_i for the polar night (PN) and polar day (PD) are given in Fig. 2. The polar night temperature ranges from -32 to 2 °C with the mean at -14 °C. In contrast, the warmer polar day varies less (-22 to 8 °C) and has a mean value of -2 °C. The vertical velocity is narrowly arranged around 0 m s^{-1} for both polar night and day, and both the polar day and polar night low variation (standard deviation: PD 0.35 m s^{-1}, PN 0.29 m s^{-1}). Extremes, which happen very rarely, are found more in the upwards motion, with the overall maximum at 6.43 m s^{-1}. The saturation with respect to ice does not reach as high values during the polar day as during the polar night.

As mentioned in Sec. 2.1, the hydrometeor types are split into frozen and liquid masses. Of the total 26.3 days of low-level clouds during the polar night, almost all contain periods with frozen hydrometeors (25.4 days), and slightly more than half

Figure 1. Processes mean values and occurrence during the polar night (a) and polar day (b). Orange crosses and text indicate processes which affect the liquid phase, and purple dots and text those which affect the frozen phase.

Figure 2. Distribution of the temperature (a), vertical velocity (b) and ice saturation ratio (c) for the polar night (red) and polar day (blue).

contain liquid hydrometeors (15.5 days, 58 %). For the 37.9 days of low-level clouds during the polar day, almost all times contained liquid (96 %) while only 31 % contained ice. This is connected to the fact that liquid occurs at higher temperatures, which are more prevalent during the polar day (Fig. 2 a). To put the process rates into context, the liquid and frozen mass mixing ratios themselves generally lie between 10^{-8} and 10^{-3} kg kg-1. Another aspect to note is that similar to Shupe et al. (2008) and as theorized by Korolev (2008), we found that higher upward vertical velocities are connected to higher saturation and with that also to higher hydrometeor masses (not shown). This already hints towards potential correlations between certain processes and the vertical wind and saturation.

3.3 Dependence on environmental conditions

An interesting aspect of microphysical processes is the circumstances under which they occur. To understand more about this, the temperature, w, S_i and S_w were used to evaluate the processes in different regimes. It is worth mentioning here that sublimation and deposition can not occur at the same time as they are calculated by the same process. The same is true for evaporation and condensation. Other processes can occur at the same time. Starting with the processes affecting the frozen mass and the temperature, it can be seen that deposition and sublimation occur relatively consistently at all temperatures below 0 °C (Fig. 3 i and j) while the mean mass change decreases (Fig. 3 c and d). For sublimation the tendency spread also increases with temperature, which cannot be seen as clearly for deposition. Another process showing a decreasing tendency with temperature is rain freezing, which occurs more often for higher temperatures, but the amount of frozen mass increases with temperature (3 f and l). Rain freezing, as expected, is more efficient with lower temperatures but has less total impact the colder it is. Interestingly, a bi-modal distribution is visible in Fig. 3 e and k for riming for both the tendency as well as the occurrence. One maxima lies below approx. -20 °C, where there are altogether few cases, and one above -10 °C. This is possibly connected to the maximum saturation difference between ice and liquid water as the cloud droplet mean mass has a local minimum of around -18 °C. Melting and evaporation, due to melting, are only active above 0 °C and decrease accordingly with increasing temperatures as less and less frozen mass is available. The homogeneous and heterogeneous ice nucleation and cloud droplet homogeneous freezing happen so rarely that they are not further included. CCN activation occurs throughout all temperatures above -34 °C but is likewise seldom, especially below -20 °C. The main processes affecting the liquid mass, as discussed above, are the processes of phase change, which affect the frozen mass, evaporation, and condensation. It is intriguing that evaporation appears to be the most prominent process throughout all temperature regimes (Fig. 3), with condensation being less prominent. On the other hand, condensation has, on average, a higher mean mass change and shows much less spread consistently throughout all temperature bins.

The next variable to look at is the vertical velocity. For the frozen mass, only three processes showed a signal; therefore, this section will focus on those. One is riming, which increases with upward velocity in occurrence. This can mainly be seen during the polar night as riming is much more frequent there (Fig. 4 b). The riming tendency may suggest an increase with upwards velocity as shown in Fig. 4 a), although the fact that only 1 % of the cases are above 1.2 m s^{-1} makes this slightly speculative.

Figure 3. Temperature dependence of microphysical processes. Left column: box plots for temperature bins. Right column: Occurrence for each temperature bin. The data includes the polar night and polar day, and bins of 2 °C are used.

If one discards the lowest and highest 1 % of the vertical wind speed, then the decrease of sublimation with upward velocity and its increases towards higher downward velocity can be seen (Fig. 5 a, white areas.). For sublimation, no difference in the behaviour between polar night and day is found. For deposition, one would expect the opposite behaviour, but as visible in 5 b), combining the polar day and polar night, such behaviour is not completely obvious. Interestingly, for deposition, a difference in its behaviour with w can be seen between polar night and polar day. The deposition frequency increases with upward velocity clearly for the polar night (Fig. 5 c). This behaviour is not so clear for the polar day (Fig. 5 d), where deposition seems common for downward motion. Additionally, the deposition rate during PD does not show a strong dependence on the vertical velocity (not shown), although previous observations show a decrease of ice mass with downward motion (Shupe et al., 2008). Reasons for this behaviour could be the lower number of frozen cases during PD or the differences in temperature range. Another reason could be differences in the vertical structure of the boundary layer and potentially increased moisture in the lower layers due to the fjord by Ny-Å. One must keep in mind that the vertical wind is very narrowly distributed around 0 m s^{-1}, and only a few absolute high values exist. To study this further, other types of clouds that have stronger vertical velocities by nature are more suitable. For the liquid mass, similarities exist between evaporation and sublimation, as both show a decrease with upward velocity. Condensation resembles the deposition more strongly and increases with upward motion. The CCN activation is, by definition, dependent on the vertical velocity. Therefore, the increase with higher upward velocity, which we found, is as expected.

The next aspect is the saturation with respect to ice and water. Processes that change the frozen mass are evaluated against S_i. Here, riming stood out again. It can be seen in Fig. 4 c and d that riming increases with saturation in both occurrence and mean tendency. This fits the increase of riming, which was described for higher upward velocities as the saturation of the rising air can increase. Some processes depend, by definition, on the saturation, for instance, deposition/sublimation and condensation/evaporation. The signal found for these processes showed evaporation and sublimation below saturation and condensation and deposition above saturation, which was, therefore, expected. What was noticeable, though, was that the tendency of condensation showed a higher mean in combination with a much smaller spread in comparison to evaporation. It was generally an interesting finding that some processes, such as condensation and rain freezing, showed much less spread in their tendency than others.

3.4 WBF in mixed-phase clouds

The introduction mentions that the Wegener-Bergeron-Findeisen process can be a reason why models have too little supercooled liquid, impacting the representation of MPCs. As shown in Kiszler et al. (2023) also in ICON-LEM, the amount of liquid-containing clouds is underestimated. Therefore, we want to go beyond evaluating single processes and demonstrate, using the WBF process, how the process rates tell us more about intertwined processes in clouds. In the previous sections, it became clear that evaporation occurs frequently. The hypothesis is that this evaporation could partially be increased as part of the WBF process. This could suppress the production of liquid in the first place or decrease the amount of liquid in a mixed-phase cloud. To see if the WBF process can be found for the data in this study, a subset containing only mixed-phase clouds

Figure 4. Dependence of riming on the vertical wind speed (left column) and the saturation with respect to ice (right column). The upper rows show the distribution of the riming tendency per bin as boxplots. The lower row shows the frequency of occurrence per bin. Bins of 0.1 are used for the saturation and 0.3 m s^{-1} for the vertical wind. The grey shaded areas indicate each the lowest and highest 1 % vertical wind speeds.

was produced (frozen mass and liquid mass both above 10^{-8} kg kg^{-1}). Then, all points where evaporation occurred were selected and split into two sets. One has cases where deposition occurs simultaneously and where it is, therefore, sub-saturated with respect to water and saturated with respect to ice. The other set has cases where no deposition occurs.

In Fig. 6 a), the distribution of the evaporation tendency for both evaporation sets is shown, and one can clearly see that they differ strongly. For the cases where deposition is happening at the same time as evaporation, the evaporation tendency is generally much larger than when no deposition is occurring. It should be kept in mind that this is a logarithmic scale, where two orders of magnitude make a large difference in the amount of liquid evaporating. In Fig. 6 b) and c), one can see the distributions of frozen and liquid masses when deposition and no evaporation is occurring and when deposition and evaporation are occurring simultaneously. Here, too, there are clear differences between the distributions, showing a shift towards higher frozen masses when deposition and evaporation occur at the same time. At the same time, the liquid mass distribution shifts towards lower values when both processes occur. In Fig. 6 c), the tail of the liquid mass, which is visible for the deposition

Figure 5. Occurrence of sublimation (a) and deposition (b-d) with vertical velocity (bin width: 0.3 m s^{-1}). Sublimation is shown for polar day and night (a), deposition for polar day and night (b), the polar day (c), and polar night (d). The grey boxes mark the lowest and highest 1 % of the vertical wind.

and evaporation cases, is due to rain, which often occurs in subsaturated layers as it falls. Combined, this demonstrates a decrease in liquid mass while there is an increase in frozen mass for cases where deposition and evaporation occur at the same time. For both Fig. 6 b) and c), we found the difference in the distributions to be statistically significant. This is also visible in the difference in mean values for both processes. When both processes occur at the same time, the average deposition rate experiences a one-order-of-magnitude increase ($9.8 \cdot 10^{-9}$ to $3.9 \cdot 10^{-8}$ kg kg^{-1}), while the average evaporation rate also increases with the same order of magnitude ($2 \cdot 10^{-8}$ to $1.3 \cdot 10^{-7}$ kg kg^{-1}). This suggests that a significant amount of water transitions from liquid to vapour and then to the frozen phase via the WBF process. It would be interesting to explore the sensitivity of the WBF process to changes in the process rates further. Such analysis is beyond the scope of this study, but it is worth noting that the developed methods are readily usable to perform such sensitivity studies.

4 Discussion and conclusions

This study evaluates the microphysical processes of the two-moment microphysics scheme from Seifert and Beheng (2006) as it is implemented in ICON. The area of focus is Svalbard, and only low-level clouds are selected for the analysis. Using a wrapper to run the microphysics scheme offline as a diagnostic tool, the process rates per timestep are written out. In total, eight months, four polar night and four polar day, are simulated. The goal is to determine which processes play the largest role in the phase transitions in Arctic low-level clouds and in what way they depend on temperature, vertical velocity and saturation.

It was found that the dominating processes are phase transitions between liquid hydrometeors and vapour, as well as frozen hydrometeors and vapour. The results suggest one possible approach to improving the representation of low-level mixed-phase

Figure 6. Histograms of the logarithm of evaporation tendency (a), frozen mass (b) and liquid mass (c). a) Liquid mass change due to evaporation in each timestep (evaporation tendency) for MPCs where no deposition occurs (orange) and where deposition occurs (green). b) Frozen mass for MPCs where deposition but no evaporation occurs (red) and where deposition and evaporation occur simultaneously (blue). c) is analogue to b) but shows the liquid mass.

clouds in the Arctic could be to adjust the processes of evaporation/condensation and deposition/sublimation. Another approach could be to increase the activity of processes which are currently less active, as these may not be active enough. Further, the differences between polar night and polar day showed the importance of evaluating a large dataset. For instance, rain freezing impacted the frozen mass during the polar day much more than during the polar night. It is worth mentioning that nucleation processes only minimally change the mass directly, but the numbers of activated CCN and INP have an impact on other process rates. Fan et al. (2017) showed this in a case study for orographic clouds where evaporation became stronger than condensation for higher aerosol concentrations, whereas for lower concentrations, the process rates were similar. Therefore, although changes to evaporation/condensation and deposition/sublimation likely will cause large hydrometeor mass changes, the interaction between processes also plays an important role.

We further explored how each process behaves in different thermodynamical regimes. Temperature is one important factor that determines the importance of a process. For instance, Fan et al. (2017) found that for warm orographic MPC riming was similarly important for the snow formation as deposition, but for cold orographic MPC deposition was clearly more important. In this study, differences are visible between the polar night and day. We found that melting and rain freezing play a larger role during the polar day while riming decreases in importance during that time. This dependence on temperature was further evaluated, and it could be seen that processes that change the mass phase between liquid and frozen show a stronger temperature dependence than those involving vapour phase transitions. The strongest temperature dependence was visible for rain freezing,

which showed an increasing occurrence with increasing temperatures, while the mean frozen rain mass decreased. Interestingly, the distribution of riming for both occurrence and mean mass change in different temperature regimes was bimodal, showing a minimum between -20 and -10 °C. The connections between the process rates and the vapour saturation and vertical wind were not as clear. This can partially be attributed to the narrow range of values for these thermodynamic variables given in low-level Arctic clouds. The clearest signal, in this respect, was the increase of riming with increasing upward velocities. This could be connected to the larger production of liquid in updrafts where the WBF process is not active (Ervens et al., 2011; Korolev, 2008).

Going a step beyond single process rates, we demonstrated how the combination of process rates can teach us more about intertwined processes. Here, we looked at the Wegener-Bergeron-Findeisen process, where liquid water evaporates and then deposits on ice due to the lower saturation of ice below 0°C. For this purpose, only mixed-phase clouds were selected. The evaporation tendency was evaluated in combination with the frozen and liquid mass, and the results suggest that a notable amount of mass follows the WBF pathway from liquid to vapour to the frozen phase. Reducing this amount may be a way to reduce the underestimation of liquid-containing clouds found in a previous study (Kiszler et al., 2023).

As stated above, there are limitations to our approach, which might make it less insightful for cases where advection dominates the cloud hydrometeor composition, for instance, in deep convective cases. Nevertheless, when focusing on low-level clouds in the Arctic, this approach provides valuable insights in regard to the processes inside the clouds, as demonstrated in this study. Additionally, the regimes of vertical velocity and temperatures studied here are limited to those of low-level clouds in the Arctic. Therefore, to create a broader picture of the microphysical processes in other cloud types, further studies, including stronger vertical velocities and larger temperature ranges, are necessary. This could, for instance, substantiate our findings in regard to the increase of riming with higher upward vertical velocities.

There are further factors that impact the process rates, as mentioned in the introduction. These include aerosol concentrations, which can strongly impact the hydrometeor composition and cloud lifetime (Kalesse et al., 2016; Eirund et al., 2019). In this study, the CCN and INP are treated as maritime, which is more accurate than the default continental setting in ICON but still not completely correct. CCNs and INPs are another large area of active research, which is why this study focuses on the processes independently of aerosol influences. An interesting study would be, though, how tweaked CCN and IN settings impact the process rates using the approach presented here. Using the process rates and looking into the regimes where different processes occur has shown that this method is also valuable for studying individual processes in greater depth. Being able to quickly change a process setting and get an idea of what might change in the model has proven easy and reliable. This encourages continuing to use tools such as this wrapper, which simplifies the untangling of complex cloud microphysics schemes.

Code and data availability. The microphysical wrapper code is stored on the DKRZ Gitlab. It includes ICON code and is therefore only available on request for anyone with an ICON license. The ICON model code is available for institutions or individuals under a licence: https://code.mpimet.mpg.de/projects/iconpublic/wiki/Howtoobtainthemodelcode. The process rates, low-level cloud selection and meteograms are available on Zenodo with the DOI: 10.5281/zenodo.10117706. A GitHub repository containing the code necessary to reproduce the results can be found here: 10.5281/zenodo.10341631

Author contributions. TK carried out the wrapper implementation, data processing, and method development, created the visualisations and prepared the manuscript with contributions from all co-authors. VS and DO contributed to the conceptualisation, research supervision, and discussion of results.

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Part IV

CONCLUSIONS AND HOW TO CONTINUE

8 CONCLUSIONS & PERSPECTIVES

8.1 SUMMARY AND CONCLUSIONS

This thesis presents three studies, all of which revolve around Arctic clouds. Three research questions were posed at the beginning of this work, and each study aimed at answering one of these.

The first research question was "*How well does ICON-LEM perform in a complex Arctic environment with respect to humidity and clouds?*". Five months of ICON-LEM simulations were evaluated against observational data to answer this. Both simulation and observation data were taken for Ny-Ålesund (Svalbard), which provides a heterogeneous terrain. It was found that the model's performance varied depending on the evaluated variable. Large-scale features such as the temperature and horizontal wind in the free troposphere were well represented. What became apparent was the strong locality of other parameters, such as the BL wind and humidity. The orography strongly impacted the BL wind, and the presence of the fjord impacted the humidity. Nevertheless, the local features could also be captured well, although details such as the exact moisture distribution were not represented as accurately. The simulated IWV showed a slight positive bias compared to the microwave radiometer HATPRO, although the mean value was slightly lower in the simulations than in the observations. Further, it was found that HATPRO became saturated towards high IWV, therefore underestimating these values compared to the IWV measured with the radiosonde. The differences between HATPRO and ICON-LEM were below 1 kg m^{-2} after accounting for the saturation of HATPRO, but it is debatable at what point the water vapour amount is captured accurately enough. As most water in the atmosphere is vapour and only small amounts are converted to liquid or frozen water, slight differences can have a significant impact. At the same time, one should not expect a model, by definition a simpler representation of a system, to capture the exact horizontal and vertical variability of the IWV. Using larger spatial domains to account for the variability of IWV would be beneficial in this respect. Satellite-based IWV retrievals, which can cover large areas, can deviate strongly in the Arctic (Crewell et al., 2021). Therefore, it is necessary to improve these large-scale observations further so that they can be used for model evaluation. When evaluating the LWP, it became clear that this is a difficult variable for the model to capture correctly. Indeed, compared to the representation of precipitation, it seems like

the LWP was worse represented in the model. Many cases where liquid water was observed showed no liquid water in the model. One factor that challenged the comparison of HATPRO observations and simulations was how to account for precipitation, as liquid precipitation causes inaccurate LWP and IWV observations. For future studies, it would be beneficial to eliminate the restrictions, although this is not trivial to achieve. While learning much about the limitations of comparing observations and high-resolution simulations, this study showed how well a state-of-the-art atmospheric model can capture such an Arctic environment. Given that this study was conducted with simulations in the grey zone of resolving turbulence, it may be unexpected that the model's overall performance was good and meaningful insights could be gained. This highlights the benefit of using a realistic setup that includes the local topography and uses NWP boundary data compared to standard (semi-) idealised LES. It further showed that the chosen resolution was suitable for the focus of this study and that using ICON-LEM gave more accurate results than ICON-NWP. Summarising, I answered the first research question by providing an overview of different variables and their representation in ICON-LEM in a complex Arctic environment.

After finding the liquid water not to be satisfyingly represented, several questions opened up about why this could be. One hypothesis was that the aerosols and nucleation/activation parameterisations were potentially a reason. This led to the second research question: "*How does a change in the INP and CCN parameterisations impact the liquid water path and supercooled liquid fraction?* To evaluate this, two months of simulations with different INP and CCN parameterisations were run and evaluated. The first simulation set used the default setting for the INP and CCN nucleation, which were originally matched to European aerosol concentrations (Hande et al., 2015, 2016). The second simulation set used maritime aerosols and a CCN activation and INP nucleation scheme from Segal and Khain (2006) and Phillips, DeMott, and Andronache (2008), respectively. The hypothesis was that using lower CCN and INP concentrations in the maritime setting might improve the representation of liquid water as they more closely match Arctic concentrations. The cloud occurrence, cloud phase, supercooled liquid fraction, IWV, LWP, IWP, and the hydrometeor number concentrations and mass mixing ratios were analysed to evaluate the impact of the chosen schemes. Overall, the largest changes could be seen for the liquid hydrometeors and, accordingly, for the LWP. While the supercooled liquid fraction was generally higher for the maritime setup, the mixed-phase cloud fraction barely changed. Additionally, the LWP decreased for the maritime setup, which matched the distribution of low LWP values better but did not capture high LWP values. The major difference came from the number of activated

CCNs and the large change in droplet numbers. The droplet number concentration decreased drastically with fewer CCN available. In line with the current understanding of aerosol-cloud interactions (Section 1.3), this caused an increase in rain droplets. If one now goes back to the discussion of the radiative effect of clouds, such changes in droplet concentrations and lower LWP can have large consequences for the radiative properties of a cloud. The assumption is that such a change would make them less optically thick and decrease their surface warming ability in the winter. Not only would it be necessary to represent liquid-containing clouds better, but the consequences on the radiative budget must be considered when choosing an aerosol and nucleation parameterisation. This said, it was decided to continue the simulations with the maritime settings, which could capture the more frequently occurring LWP values (<500 g m^{-2}) more accurately when using HATPRO as the reference. The entire study clearly shows a strong need to improve the representation of Arctic aerosols in ICON, and how this could continue is discussed in the next section. Another conclusion of this study was that although the INP and CCN strongly impact the cloud properties, especially the liquid, other factors must impact the MPC occurrence more as it barely changed.

The conclusions of the previous study led me to the third research question: *Which microphysical processes dominate the phase-partitioning in low-level Arctic clouds?* This opened up exciting terrain where the microphysical processes are directly evaluated. To achieve this, a method had to be found to write out the microphysical process rates. One possibility was to write them out during the simulations directly, but as the output of many simulations already existed, the wish was to use the existing data. Therefore, I implemented a "microphysical wrapper" which enables the running of the saturation adjustment and the two-moment scheme by Seifert and Beheng (2006) as a diagnostic tool. Eight months of simulations were selected, and a subset only consisting of low-level clouds (cloud top <2.5 km) was created. As there are distinct differences between the polar night and day, the next step was to differentiate between these two periods. Then, the microphysical processes which contributed to the phase changes were evaluated. While there were apparent differences between both periods, for instance, showing less frequent sublimation during the polar day while rain freezing, and melting became more relevant, some common features existed. Evaporation generally has the greatest impact on liquid water and the majority of phase changes occur through the vapor phase. The processes were further evaluated for different temperature, saturation and vertical velocity regimes. There, it could be seen that the temperature had the most considerable impact on the process rates. Local features of Ny-Ålesund, such as the fjord, also seem to influence the process rates. For instance, evaporation in

clouds might dominate over the land because the advected moisture from the fjord is confronted with the dryer air over land. The choice of analysing low-level clouds influenced the vertical wind selection as the low variability limited the meaningfulness. Generally, it can be argued that the resolution, although in the grey zone of turbulence, is a good choice as the models that use such two-moment schemes can have much lower resolutions and will be even less able to represent the vertical motion. Another aspect that was evaluated as part of the interest in the cloud phase-partitioning was the WBF process. A significant amount of liquid was found to transition to frozen particles via the vapour phase. This potentially hints towards the need to rethink how the homogeneous representation of liquid and ice in the same grid box could be represented as a more heterogeneous distribution to avoid glaciation where there should be none. Combining improved aerosol representation with a direct look at the microphysical process rates will be necessary to better understand how changes to each process will impact the other processes. Ultimately, these findings for cloud-resolving simulations can also benefit climate models and bring us towards a better representation of Arctic clouds.

8.2 PERSPECTIVES

The findings of this thesis bring considerable potential for further research. There are different aspects that I will discuss here. The first one is the representation of aerosols in models. There are two sides to this, one is the observations and one is the models. We still lack observations, although there are ongoing efforts to address this through long-term measurements and campaigns. Such observations are necessary to create Arctic aerosol profiles, which can be used to constrain model parameterisations. In models, it has to be considered if there are ways to better capture the variability of the aerosols and the regions' specific profiles. A conceptual suggestion to include aerosol variability in a new INP parameterisation was recently presented by Frostenberg et al. (2023). Although the presented parameterisation did not give better results in a cloud model than a more established INP parameterisation based on Fletcher (1962), exploring such approaches is worthwhile and necessary.

The second aspect is understanding how microphysical processes influence each other and how they are implemented. In an attempt to quantify how a change in one process may affect other processes, a first analysis has been made by adapting the water diffusion function. This showed that a minor change in one process will cause the majority of the other process rates to change. One can get a feeling for these changes and potentially establish correlations between different processes using the microphysics wrapper. If shown to be impactful

in the wrapper, such changes can be studied using adapted simulations. This way, one could try to untangle the interactions of the processes. Examples of such changes are adaptations to the CCN and INP parameterisations or to the water diffusion, which impacts the deposition and sublimation rate. A lot of data already exists, and it is possible to create statistical studies to develop and improve cloud microphysical parameterisations based on this data. This thesis is an example of how we can step away from using single cases and instead use several months with the given computational resources. With the current high-performance computing resources, approaches using many simulations or large simulation domains representing varying real-life conditions should be strived for. While using a small number of cases remains valuable for testing or when working on specific field observations, improvements made to models to best represent the selected cases often reach a limit when put to the test in different conditions.

Additionally, it may be worth rethinking how we implement cloud microphysical parameterisations. One can choose from certain predefined sets of parameterisations, e.g., the SB06, in ICON. Instead of implementing entire schemes to choose from, one could implement several versions of each process and let the user decide which ones to use while providing a default setting. Some basic assumptions would have to be made, such as how many moments one computes and how many hydrometeors one uses. Otherwise, processes cannot be combined with each other. Being able to choose so freely makes comparisons more difficult if everyone uses slightly different settings, but it lets us face the problem as it is. Microphysical processes are complex, and one often doesn't know which difference in the parameterisation causes the difference in the simulation output if the entire microphysics scheme has been changed. Going away from whole microphysics scheme switches, one could make simulations with the underlying base assumptions (i.e. the number of moments, hydrometeors, etc.) actually more straightforward to compare. One can also use the best of each parameterisation because none is perfect. One could potentially also tune the parameterisation better for regional modelling. One could create differently tuned process representations depending on the climate zone and let the user decide whether to use these because tuning will still have to happen. Developing a model using such a modular approach can also be simpler, although a test suite to run all parameterisation function combinations would be required. And yes, adding an extra namelist with all types of settings for the clouds and reimplementing the microphysics may seem like a lot, but in the face of this being one of the largest uncertainty sources in climate models, I believe it is worth the effort.

Besides different approaches to parameterisation implementation, it is worth exploring alternative approaches such as machine learning. Although machine learning currently cannot fix the inherent problem of cloud microphysics, as it learns from existing models, it is possible to use these techniques to make sense of the complex interactions between processes or, as suggested by Couvreux et al. (2020), to tune models. This could help in combining observational data with the models. For example, the steadily improving remote sensing, which can be directly compared using forward modelling, shows some potential to exploit. A recently installed polarimetric K-band radar at Ny-Ålesund is an example of how we can now gain more insights into particle shapes and sizes. Such observations can be used to constrain the microphysical parameterisations better. It could also be imaginable that only parts of the parameterizations are replaced with ML methods. For instance, replacing more uncertain processes with neural networks that can be trained so that the output matches the observations better.

As a last aspect, I would like to mention that to represent clouds, not just the microscale plays a role but also large-scale processes. Overall, the limited area simulations performed well when the large-scale features had already been captured accurately by the NWP model. If the NWP model already failed to capture the synoptic situation, the limited area model also failed. Further, the shift towards hectometer scale simulations opens up the need for turbulence parameterisations, which are more flexible and can cover the gap between RANS and LEM simulations. Therefore, the challenge of correctly representing clouds is not just limited to the microphysics and aerosols but also requires looking at other model components. In the end, using all available tools and connecting observations with simulations where that can be done will really bring us forward.

DECLARATION

Hiermit versichere ich an Eides statt, dass ich die vorliegende Dissertation selbstständig und ohne die Benutzung anderer als der angegebenen Hilfsmittel und Literatur angefertigt habe. Alle Stellen, die wörtlich oder sinngemäß aus veröffentlichten und nicht veröffentlichten Werken dem Wortlaut oder dem Sinn nach entnommen wurden, sind als solche kenntlich gemacht. Ich versichere an Eides statt, dass diese Dissertation noch keiner anderen Fakultät oder Universität zur Prüfung vorgelegen hat; dass sie - abgesehen von unten angegebenen Teilpublikationen und eingebundenen Artikeln und Manuskripten - noch nicht veröffentlicht worden ist sowie, dass ich eine Veröffentlichung der Dissertation vor Abschluss der Promotion nicht ohne Genehmigung des Promotionsausschusses vornehmen werde. Die Bestimmungen dieser Ordnung sind mir bekannt. Darüber hinaus erkläre ich hiermit, dass ich die Ordnung zur Sicherung guter wissenschaftlicher Praxis und zum Umgang mit wissenschaftlichem Fehlverhalten der Universität zu Köln gelesen und sie bei der Durchführung der Dissertation zugrundeliegenden Arbeiten und der schriftlich verfassten Dissertation beachtet habe und verpflichte mich hiermit, die dort genannten Vorgaben bei allen wissenschaftlichen Tätigkeiten zu beachten und umzusetzen. Ich versichere, dass die eingereichte elektronische Fassung der eingereichten Druckfassung vollständig entspricht.

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Theresa Kiszler

DATA AND CODE AVAILABILITY

For this thesis, simulation data and code were created. A list of where to find these is provided here. Not all code can be made public, but this is commented on accordingly.

ICON code is available under a license: https://code.mpimet.mpg.de/projects/iconpublic/wiki/Howtoobtainthemodelcode

First study
GitHub repository for code:
https://github.com/TracyMcBean/kiszler_et_al_2023_code
Data available on DKRZ long-term storage:
hdl:21.14106/caa5a96169e6149e029fed49157b117599a959ae

Second study
GitHub repository for code:
https://github.com/TracyMcBean/ccn_inp_impact_on_clouds
Data available on Zenodo: 10.5281/zenodo.10400633, 10.5281/zenodo.10400648

Third study
GitHub repository for code:
https://github.com/TracyMcBean/Kiszler_et_al_2023_microphysics
The microphysical wrapper code is available on the Gitlab of the Deutsches Klimarechenzentrum (DKRZ, German climate computing centre). It can be accessed by those who have an ICON license.
Data available on Zenodo: 10.5281/zenodo.10117706

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Part V

APPENDIX

A APPENDIX

A.1 TECHNICAL DETAILS OF THE MICROPHYSICS WRAPPER

In this section, further technical details of the microphysics wrapper, introduced in Section 4.3, are provided. To run the microphysical scheme outside of ICON, the code for the two-moment microphysics scheme and additional required modules had to be separated from the rest of the model code. Several modules had to be added to create a working interface between the ICON output and the microphysics driver. All data is expected to be given and will be stored following the NetCDF format[1]. To achieve this, the following modules were added:

`run_2mom_wrapper.f90`: Main file to run the wrapper. Here, all functions are called, and the actual interface is provided for the saturation adjustment and the 2-moment microphysical scheme. The interface to the main function `two_moment_mrcph()` is further explained in the schematic in Figure 14.
`mo_2mom_wrapper_types.f90`: Contains the routines to create variable types compatible with ICON and to allocate memory for the variables.
`mo_2mom_wrapper_util.f90`: This file contains all subroutines needed for I/O, getting the layer depth and the information about the input file dimensions.
`mo_2mom_wrapper_namelists.f90`: Reads in the namelists and assigns variable values accordingly. Namelist settings include the filenames for the in and output (`infile, outfile, tendfile`), the message level (`msg_level`), the choice of microphysics (`inwp_gscp`, timestep (`dtime`), input format (`input_3D`), potential array size for splitting (`max_ncells`), and the variable names in the input file (`invar_names`). A default namelist is provided as an example (`run/namelist_default.nml`).

The wrapper can be built using `make`, and several namelist options are available to select the input and output files, provide the variable names, and the data format (2D or 3D). The possible input names are given in Table 2. The output contains 69 variables: the hydrometeor masses and their tendencies after each timestep. The tendencies are listed in Table 3.

1 https://www.unidata.ucar.edu/software/netcdf/; Accessed: 13.10.2023

Figure 14: Interface to the 2-moment microphysics subroutine `two_moment_mcrph()` as implemented in ICON used in the wrapper with indications of which variables are used at which timestep and what has been added.

NAME IN CODE	DESCRIPTION	POSSIBLE INPUT NAMES
narr	Number of arrays (columns), will be number of cells for 3D input and 1 for meteogram input	ncells
pres	Pressure	pres, pressure, PRES, Pressure, P
temp	Temperature	temp, temperature, TEMP, Temperature, T
rho	Density	rho, RHO, density, DENSITY, Density
qv	Specific humidity	qv, QV
qc	Specific cloud water content	qc, QC
qnc	Number concentration cloud water droplets	qnc, QNC
qr	Rain mixing ratio	qr, QR
qnr	Number concentration rain droplets	qnr, QNR
qi	Specific cloud ice content	qi, QI
qni	Number concentration ice	qni, QNI
qs	Snow mixing ratio	qs, QS
qns	Number concentration snow	qns, QNS
qg	Graupel mixing ratio	qg, QG
qng	Number concentration graupel	qng, QNG
qh	Hail mixing ratio	qh, QH
qnh	Number concentration hail	qnh, QNH
inact	Number concentration activated ice nuclei	inact, INACT, NIACT, niact, ininact, ININACT, ninact, NINACT
w	Vertical wind	w, W, omega, OMEGA
hhl	Half level height	hhl, HHL, height_2
fhl	Level height	fhl, FHL, height

Table 2: Variables needed as input for the microphysics wrapper.

PROCESS	CLOUD DROPLET	RAIN	ICE	SNOW	GRAUPEL	HAIL	SPEC. HUMIDITY
Evaporation & condensation	+/-						+/-
Autoconversion	-	+					
Rain evaporation		-					+
S/G/H evaporation				-	-	-	+
Droplet homog. freezing	-		+				
Homog. & heterog. freezing	-		+				-
Riming	-	-	+	+	+	+	
Frozen collisions (excl. hail)			-	+/-	+		
Graupel to hail					-	+	
Hail collisions			-	-		+	
Rain freezing		-	+		+	+	
Ice melting	+	+	-				
Snow, graupel, hail melting		+		-	-	-	
Deposition & sublimation			+/-	+/-	+/-	+/-	+/-
CCN activation	+						-

Table 3: Processes included in the wrapper's output, including their impact on the mass mixing ratios of each hydrometeor type (+ increase, - decrease). The hydrometeors are cloud droplets, raindrops, ice particles, snow particles, graupel, hail and the specific humidity q_v. Processes with a plus and minus (+/-) can increase or decrease the mass.

A.2 SUPPLEMENT TO CHAPTER 6

The following figures (Figure 15 and Figure 16) show further analysis on comparing the Hande and SK-P parameterisations schemes, which complements the presented analysis in Chapter 6.

Figure 15: Vertical distribution of the hydrometeor mass mixing ratios in August and October 2021 for cloud droplets (a), rain (b), graupel (c), snow (d) and cloud ice (e). Note that differing y-label extents. The dashed lines show the median, the solid lines show the mean, and the interquartile ranges (IQR) are marked by the shaded areas. Blue colours are for the Hande simulations, and red is for the SK-P simulation.

Figure 16: Vertical distribution of the hydrometeor number concentrations in August and October 2021 for cloud droplets (a), rain (b), graupel (c), snow (d) and cloud ice (e). Note that differing y-label extents. The dashed lines show the median, the solid lines show the mean, and the interquartile ranges (IQR) are marked by the shaded areas. Blue colours are for the Hande simulations, and red is for the SK-P simulation.

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