A case study of frontal cloud microphysics in model and observations

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Abstract

Cloud microphysical parameterizations in weather and climate models have continuously increased in complexity to better represent the variety of underlying cloud processes. This study tests how well the current two-moment microphysics scheme of the Icosahedral Nonhydrostatic Model (ICON) performs when compared to observations. As a comparison, in-situ and remote sensing observational data from the North Atlantic Waveguide and Downstream impact Experiment (NAWDEX) are used to identify the properties of a mid-latitude frontal cloud. In addition to investigating the holistic behaviour of the cloud microphysics, a special focus is also placed on the scheme’s ability to correctly predict ice particles through homogeneous nucleation. Within the framework of this case study, the model shows an overall good consistency in terms of water content, relative humidity and particle size distribution. Larger deviations from the observations are found, especially at high altitudes where ICON overestimates the relative humidity and underestimates the number density of small particles. Sensitivity tests show that the reason for the deviations is found in the parameterization of homogeneous ice nucleation, i.e. an inbuilt humidity threshold variable that prohibits the scheme from being activated. Only strong reductions of this threshold value lead to a realistic number of small ice particles. The results suggest that sub-grid scale humidity fluctuations are the likely cause for the threshold value not being reached. This hypothesis is supported by the fact that the model shows an increase in small ice particles at weaker threshold reductions when run at a higher spatial resolution. Though there is strong evidence for this assumption, further analysis of the nucleation behaviour for increasingly small grid sizes is critical to substantiate the hypothesis.
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1 Introduction

Clouds play an important role in influencing atmospheric circulation and the climate system as a whole (Bony et al., 2015). Nevertheless, cloud radiative effects of aerosol–cloud interactions are subject to large uncertainties as sub-grid scale parameterizations in weather and climate models are often not able to accurately represent all relevant processes (Boucher et al., 2013). Thus, great effort is put into tackling such uncertainties by increasing the complexity of the parameterizations. With a constant gain in computing power, increasingly more physical processes can be included that in the past were oversimplified or neglected. This is especially true for cloud processes that often occur at scales too small for common climate or weather models to calculate directly. However, this does not necessarily mean that more complex parameterizations automatically lead to a more realistic representation of clouds.

As parameterizations evolve, there is a need for constant evaluation. This study chooses to investigate how realistic the current two-moment cloud microphysics scheme (Seifert and Beheng, 2006) that is implemented in the Icosahedral Nonhydrostatic Model (ICON; Zängl et al., 2014) is when compared to observations. However, clouds are complex and nonlinear phenomena, and their properties depend on many variables such as the ambient temperature or the cloud type. Therefore, the analysis is simplified by regarding only a single cloud in a case study. Such an opportunity arose during one day of the North Atlantic Waveguide and Downstream impact Experiment (NAWDEX; Schäfler et al., 2018) measurement campaign in 2016, where multiple aircrafts took in-situ and remote sensing measurements of an occluded frontal cloud that reached over 8 km altitude. One of the aircrafts descended through the entire cloud, allowing an examination of the cloud properties at different heights. This allows the investigation of the holistic behaviour of the microphysics scheme in this particular case study. For the analysis, the initial leading questions are:

- Is the general representation of water content and particle size distribution accurate?
- Is the distribution of liquid and frozen hydrometeor content similar to the measurements, i.e. their distribution in height?
- Does the simulated humidity throughout the cloud correspond to the measurements?

As the questions above are being addressed, it will be shown that there are significant deficiencies in the parameterization which models small ice particles at high altitude. Therefore further analysis focuses on the process that is assumed to be the main driver of these shortcomings: the homogeneous nucleation of the ice particles.

Investigating the mechanism of homogeneous nucleation (i.e. the model parameterization) is somewhat easier than investigating other cloud mechanisms. The theory is well understood, especially compared to heterogeneous nucleation that can result from a range of different
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processes and ice nuclei (e.g. Heymsfield et al., 2017) or to other mechanisms in the mixed-phase regime of clouds that depend on several different processes (Seifert and Beheng, 2006). A sensitivity study on different parameters within the homogeneous nucleation scheme is conducted to help understand why the model calculates high-altitude ice particles incorrectly. Furthermore, an analysis of two different model resolutions allows an investigation of a possible dependence of the scheme performance on the model gridsize. For the analysis of the homogeneous nucleation parameterization the following questions are used as a guideline for the investigation:

• Is the homogeneous nucleation scheme the main driver for the inaccurate representation of high-altitude ice particles in this case study? If so, what is the cause of the scheme to falsely predicting the ice particles?

• Can the ice particle size distribution be modelled correctly if the scheme is tuned? And if so, how strong does this tuning have to be and which parameters have to be changed?

• Could there be any other possible causes of the model behaviour?

The outline for this work is as follows. Chapter 2 presents the measurement data used for evaluation, the model settings and the methods used throughout the analysis. This chapter also provides background knowledge on homogeneous nucleation and its parameterization in the model. Thereafter, the model is evaluated by analysing zing water content, relative humidity and particle size distributions for all heights of the cloud in Chapter 3. This chapter also contains sensitivity studies for the homogeneous nucleation parameterization. The study is concluded in Chapter 4.
2 Data and Methods

2.1 Measurement data

2.1.1 NAWDEX campaign: The joint flight

Data from the North Atlantic Waveguide and Downstream impact Experiment (NAWDEX; Schäfler et al., 2018) campaign was chosen for as comparison for the model output as it offers a large range of airborne measurements for investigating different cloud properties. On 14 October 2016, three aircrafts equipped with in-situ and remote sensing measurement devices simultaneously took measurements of a frontal cloud northwest of Scotland. This part of the campaign is also referred to as the 'joint flight' or IOP 11 (Intensive Observation Period 11). For this work, the in-situ data that was obtained by the Facility for Airborne Atmospheric Measurements (FAAM\(^1\)) aircraft is predominantly used for analysing the microphysical cloud properties. The observations obtained by the High Altitude and Long Range Research Aircraft (HALO\(^2\)) and the Service des Avions Francais Instrumentations pour la Recherche en Environnement (SAFIRE\(^3\)) Falcon 20 are also useful as they give a larger view of the cloud. However, the only remote sensing observations used in this study are radar data from the HALO aircraft. Other studies exploiting the possibilities of this multi-instrumental observation have also been conducted (e.g. investigating the effect of different cloud particle habits on cloud radar retrieval; Duscha, 2018). By ascending through the cloud, the FAAM aircraft was able to gather in-situ measurements from different heights, allowing for a better view of the distribution and hydrometeor type of particles.

2.1.2 Synoptic situation - Overview of observed cloud

Subject of this investigation is an occluded frontal cloud that formed in the Northwest of Scotland on the 14 October 2016. Figure 1a shows that the frontal structure evolved to the north east of a low pressure system with a core location west of Ireland. Since the winds came from a predominately south-eastern direction and the front extended in the same direction, the frontal structure stayed stationary for several hours. This was supported by a low pressure system that had been cut off and was contrasted by a strong high pressure system over Scandinavia (Figure 1c). In addition, a stationary ridge over Eastern Europe was blocking the cut-off low from travelling further eastward. The occluded front presumably developed as a result of positive vorticity advection on the north-eastern side of the cut-off. As a result, a band of clouds covering most of Scotland at approximately 12 UTC (Figure 1b) occurred that extended high enough to be clearly seen on infrared satellite pictures (Figure

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\(^1\)See [https://www.faam.ac.uk/](https://www.faam.ac.uk/).

\(^2\)See [https://www.halo.dlr.de/](https://www.halo.dlr.de/).

2. DATA AND METHODS

1d). The joint flight experiment was therefore executed on a north-to-south leg to investigate the frontal cross-section.

![Surface pressure map](image1)

![Flight track](image2)

![Geopotential height](image3)

![Infrared satellite imagery](image4)

**Figure 1**: (a) Surface pressure map from the UK Met Office on 14 October 2018, 12 UTC. The red circle indicates the occluded front that is analysed in this study. Map taken from [www.wetter3.de](http://www.wetter3.de), accessed 07.10.2018. (b) Flight track of the FAAM aircraft (orange line). Satellite image is Modis corrected reflectance from the NASA Terra satellite for 14 October 2018, 12.30 UTC. All three aircrafts aligned for the 'joint flight' on the N-S section between 56N-60N (red line). Satellite image taken from [https://worldview.earthdata.nasa.gov](https://worldview.earthdata.nasa.gov), accessed 07.10.2018. (c) Distribution of geopotential height at 500 hPa (coloured contours) and surface pressure (white lines). Map taken from [www.wetterzentrale.de](http://www.wetterzentrale.de), accessed 07.10.2018. (d) shows an infrared (IR) satellite imagery from SAT24-EISQ51 over Europe at 12:00 UTC for 14th October. Image taken from [www.sat24.com](http://www.sat24.com), accessed 07.10.2018.

2.1.3 Instruments on the FAAM aircraft

The in-situ measurements obtained by the FAAM aircraft are used to obtain detailed information on the cloud microphysical properties. Especially measured number density
concentration and cloud water content are used extensively to evaluate ICON’s 2-moment scheme. The following paragraphs describe the instruments on the plane and offer a short insight into their functioning.

Cloud imaging probes

Particle data from two cloud imaging probes (CIP; Droplet Measurement Technologies, Inc., 2012) that were mounted onboard of the FAAM aircraft are available for this study. Both probes are single particle array probes with grayscale imaging capability. Each of them contains a linear array of 64 photodetectors, that measure the shadowing of a laser beam by a particle. By measuring at a higher-than-airspeed frequency, an image of the particle can be made. The CIP-15 probe measures at a resolution of 15 µm, detecting particles from a range of 15 µm to 930 µm. The CIP-100 probe measures larger particles at a resolution of 100 µm, detecting particles from a range of 100 µm to 6200 µm. Both probes return the cumulative number of particles of each size in 62 bins as 1-second averaged values of the maximum diameter. The processing algorithm rejects all particles if they result from the shattering of larger particles, are out of focus or extend beyond the edge of the imaging arrays (pers. comm. Stuart Fox, 2018). In addition to determining the size distribution, the probes also provide particle images at 15 µm and 100 µm resolution that can help identify the type and shape of the hydrometeors.

Cloud droplet probe

Particles smaller than 15 µm are measured with the cloud droplet probe (CDP; Droplet Measurement Technologies, Inc., 2013). This measures cloud droplet size distributions between 2 µm and 50 µm. Unlike the CIP devices, the CDP probe determines the dimensions of a particle by illuminating it with a laser and recording the scattering of the light that reaches the detectors on the opposite side. Depending on the scattering angle, position of the particle in the probe and intensity of the scattered light beam, the particle size is calculated and categorized according to one of 30 sizing bins. As for the CIP data, the CDP data is 1-second averaged. Since the CDP is primarily developed for cloud droplets, the size of ice and snow particles determined by the probe is rather uncertain (pers. comm. Stuart Fox, 2018), as the complex shape of frozen particles result in a different scattering of the laser beam.

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4 For affiliations of those mentioned, see Acknowledgements.
2. DATA AND METHODS

Nevzorov probe

The Nevzorov probe\(^5\) contains two separate hot-wire probes that measure liquid water content (\(LWC\)) and total water content (\(TWC\)). The resulting ice water content (\(IWC\)) is simply calculated as the difference between \(LWC\) and \(TWC\):

\[
IWC = TWC - LWC.
\]

Korolev et al. (1998) estimate an absolute accuracy of 10% to 15% for liquid drops in the size interval 10-50 \(\mu m\) at airspeed 100 ms\(^{-1}\) and 1000 mb pressure, but emphasize that the accuracy is highly dependent on the cloud microstructure and the result can therefore vary for different altitudes and airspeeds. It also should be noted that the LWC sensor has a small response in the presence of ice (pers. comm. Stuart Fox, 2018). Therefore the IWC measurement in mixed-phase clouds might be slightly biased.

Other FAAM measurements

Data on aircraft position and velocity is provided by the GPS-aided Inertial Navigation system (GIS\(^6\)) with a frequency of 32Hz. Temperature, pressure and humidity data were provided by the Tropospheric Airborne Meteorological Data Reporting (TAMDAR\(^7\)) measurement system.

2.1.4 HAMP radar on the HALO aircraft

For the short comparison of model output to observations in Section 2.2.5, the radar reflectivity from the HALO Microwave Package (HAMP; Mech et al., 2014) is displayed. The HAMP radar was mounted on board of the HALO aircraft and was operated at a frequency of 35.6 GHz (Ka-band). For more information on the HAMP radar properties and evaluation during the 'joint flight’, see Duscha (2018).

2.2 The ICON model

2.2.1 General setup and experiment design

The model used for this investigation is the Icosahedral Nonhydrostatic Model (ICON; Zängl et al., 2014) which is run in numerical weather prediction mode (NWP). It was co-developed by the Max-Planck-Institute for Meteorology (MPI) and the German Weather Service (DWD).

\(^7\)See https://old.faam.ac.uk/index.php/science-instruments/primary-systems/579-tamdar.
One of the differences of ICON compared to most other global models is the fact that it runs on an unstructured icosahedral-triangular grid instead of the more usual rectangular grid. This allows for multiple improvements, such as an easy change of resolution (e.g. for flexible one- and/or two-way grid nesting) and better scalability on parallel high-performance computing architectures (Zängl et al., 2014).

For this experiment the model was run on a horizontal resolution of roughly 2.5km, with the simulated domain covering the area over the northern Atlantic from 30°W to 15°E and 40°N to 70°N. Over the joint flight area an additional one-way nest at double the resolution was implemented from 17°W to 7°E and 50°N to 66°N. An overview of the Domains is provided in Figure 2.

![Figure 2: Model Domain Area. Outer red square marks boundaries of the larger ICON model domain at 2.5km resolution (Domain 1). Inner red square marks boundaries for the ICON nest at 1.2km resolution (Domain 2). Orange line shows FAAM flight track.](image)

The vertical resolution of the model consists of 75 levels, but contrary to many other models such as ECHAM6.3 (Stevens et al., 2013), ICON uses a hybrid sigma height grid (Giorgetta et al., 2018) instead of a hybrid sigma pressure grid. Thus the lower height levels are not vertically uniform but instead vary in height depending on the height of the orography beneath them. The levels are designed however to quickly and smoothly transition into uniform heights. This is intended to improve the coupling with planetary boundary schemes.

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8Hybrid sigma pressure levels also take the orography into account but depend on the surface pressure instead of the surface height (e.g. Retsch et al., 2017).
while retaining the advantages over classic sigma coordinates at upper levels (Leuenberger et al., 2010).

The model run was initialized for 13 October 2016 at 00 UTC and was carried out until 15.10.2016 at 00 UTC, resulting in 48 simulated hours. Therefore, the IOP occurred roughly 36 hours after the initialization. During the time of the IOP, the variable output interval was increased from one hour to 10 minutes to minimize lead-lag errors between model and observation. The model used boundary data from the Integrated Forecasting System (IFS; European Centre for Medium-Range Weather Forecasts\(^9\)) forecast at 16 km horizontal resolution (T1279), that was updated every three hours.

### 2.2.2 The Two-Moment Microphysics scheme

In order to be able to interpret the results of the model accurately, it is important to acquire some background knowledge of the underlying cloud microphysics scheme. In this study, ICON was run with a two-moment cloud microphysics parameterization based on the work of Seifert and Beheng (2006). The novelty of this scheme compared to one-moment schemes is that it explicitly calculates the evolution of both mass \(L\) and number density \(N\) of the particles. Both are moments of their particle distribution \(n(D)\), where \(D\) is the particle diameter. The number density \(N\) is the zeroth moment:

\[
N = \int_0^\infty n(D_x)dD_x
\]

and the water content \(L\) is the third:

\[
L = \frac{\pi}{6}\rho_w \int_0^\infty n(D^3_x)dD_x,
\]

where \(x\) denotes the particle type and \(\rho_w\) the density of water (e.g. Straka, 2009, chap. 2).

An important advantage of this approach is that the activation of cloud nuclei can now be included into the set of parameterized processes (Seifert and Beheng, 2006). Although spectral bin microphysics do outperform bulk microphysical parameterisations as they describe microphysical processes with more consistent accuracy, bulk microphysical parameterisations are still widely used because of their high computational efficiency (e.g. Seifert et al., 2005; Khain et al., 2015). Other attempts to improve parameterisations move towards including a third moment, which is usually the sixth moment of the distribution and is related to the reflectivity (e.g. Milbrandt and Yau, 2005; Loftus et al., 2014), or increasing the number of hydrometeor categories (Straka and Mansell, 2005).

In this scheme the mass and number density of six different hydrometeors are calculated: cloud drops, cloud ice, raindrops, snow, graupel and hail. This is done by predicting nucleation and growth of the hydrometeors as well as taking into account the transition to different

\(^9\)See also https://www.ecmwf.int/en/forecasts/.
hydrometeors independently (e.g. by melting or freezing) or as a result of the interaction of two (same or different) hydrometeors (e.g. by riming, aggregation or self-collection). Hydrometeors are eventually removed by evaporation or, naturally, sedimentation.

2.2.3 Ice nucleation and its implementation in ICON

In nature, ice particles are formed in two different ways: by homogeneous and heterogeneous nucleation. While heterogeneous nucleation uses an ice nucleus (IN) to form an ice particle by multiple possible processes such as immersion/condensation freezing or deposition nucleation, homogeneous nucleation occurs without interaction with a foreign particle within pure cloud drops or pure solution aerosol particle (Heymsfield et al., 2017, chapter 2). As this study will focus on homogeneous nucleation, the following chapters will explain the principle processes of homogeneous nucleation and how they are implemented in ICON.

Homogeneous nucleation

Regardless of the freezing temperature of water at 0°C, supercooled water droplets can exist at temperatures far below this. Between 0°C and -38°C droplets usually freeze due to heterogeneous nucleation. If there is a lack of sufficient ice nucleating particles, cloud droplets will finally freeze at -38°C due to homogeneous nucleation (Kärcher and Seifert, 2016). Below this temperature, liquid water drops cannot form anymore since the relative humidity necessary for the ice formation is below the relative humidity needed for liquid water saturation (Heymsfield and Miloshevich, 1993; Heymsfield et al., 2017). In order for an ice particle to be formed from a water drop, a critical energy barrier has to be overcome first, which is also the reason supercooled drops do not freeze as soon as they are cooled below 0°C (Cantrell and Heymsfield, 2005). Often, aerosol particles function as (heterogeneous) ice nuclei, lowering the energy barrier by acting as a catalyst and therefore allowing for droplets to freeze at higher temperatures (e.g. Murray et al., 2012). The nucleation of ice particles is assumed to be very similar to the nucleation of water droplets so that the classical theory of homogeneous nucleation can help quantify the energy barrier and understand how the nucleation works in general (for a more detailed description, see Pruppacher and Klett, 1997 or Wang, 2013.)

At temperatures of -38°C and below, it is assumed that within the water droplet, a cluster of molecules forms as a result of stochastic events. This cluster is referred to as an 'i-mer embryo' (consisting of i molecules). This embryo will then function as a nucleus for the droplet. By taking into account the Helmholtz free energy and the Kelvin law, Pruppacher and Klett (1997) derive an analytical expression for the number density of i-mer embryos $N_i$

$$N_i = N_{sat} \exp \left( \frac{-\Delta F_i}{kT} \right),$$  

(4)
where \( N_{\text{sat}} \) is the total number of molecules, \( \Delta F_i \) the free energy of formation of the \( i \)-embryo, 
\( k = 1,38 \cdot 10^{-23} \) J/K the Boltzmann constant and \( T \) the temperature. As can be seen in Equation 4, the number density of \( i \)-mer embryos resulting from homogeneous nucleation increases with reduced free energy \( \Delta F_i \) or as a result of a lower temperature. Furthermore, the free energy \( \Delta F_i \) can be expressed as

\[
\Delta F_i = 4\pi a_i^2 \sigma - \frac{4\pi a_i^3}{3\nu_{\text{mole}}} kT \ln S_{v,w},
\]

with \( a_i \) being the radius of the \( i \)-mer embryo, \( \sigma \) the surface tension, \( \nu_{\text{mole}} \) the volume of each individual molecule and \( S_{v,w} \) the saturation ratio of moist air with respect to a plane water surface. Equation 5 shows that the free energy needed to form a \( i \)-mer embryo is controlled by two adversary terms. The first term on the right side of the equation is the surface energy. It states that smaller radii and therefore fewer molecules are energetically preferable. By itself, the term would have the consequence, that a spontaneously formed embryo would shrink rather than grow. This term is contrasted by the second term on the right side of the equation. It states that the free energy reduces with increasing radii, temperature and saturation ratio. The ratio of \( a_i^2 \) in the first term to \( a_i^3 \) in the second term, has the consequence, that for small \( a_i \), the first term dominates, which results in a positive \( \Delta F_i \). For larger \( a_i \), the second term dominates and results in a negative \( \Delta F_i \). Thus, from a critical radius \( a_{i,\text{crit}} \) onward, it is thermodynamically favourable to grow. By setting the result of the derivative of Equation 5 to zero, the critical radius can be expressed as

\[
a_{i,\text{crit}} = \frac{2\pi M_w \sigma}{RT \rho_w \ln S_{v,w}},
\]

with the molecular weight of water \( M_w \), \( R \) the universal gas constant and the density of water \( \rho_w \). Further inserting Equation 6 into Equation 5 results in

\[
\Delta F_{i,\text{crit}} = \frac{16\pi M_w^2 \sigma^3}{3(RT \rho_w \ln S_{v,w})^2}.
\]

\( F_{i,\text{crit}} \) is the size of the energy barrier that has to be overcome in order for the embryo to grow. Equation 7 shows, that a higher saturation ratio reduces the energy barrier, and since the nucleation rate \( J \approx J_0 \cdot N_i \) (e.g. Cantrell and Heymsfield, 2005, Wang, 2013), this also leads to a higher nucleation rate. \( J_0 \) (units \([s^{-1} \, cm^{-3}]\)) is the net rate at which an embryo of critical size gains one molecule by colliding with surrounding water vapour molecules.

Homogeneous nucleation does not only occur in pure water droplets. Soluble aerosol particles that are the basis of more (e.g. in Cirrus) or less concentrated solutions (e.g. in convective updrafts) can also serve as a foundation for nucleation (Cantrell and Heymsfield, 2005). Although a solute does alter the freezing point (see e.g. Sassen and Dodd, 1988 for a mathematical description of the freezing point depression), it is assumed that the nucleation rate is independent of the nature of the solute, but depends only on the water activity (ratio between the water vapour pressure of the solution and pure water, Koop et al., 2000).

10
The soluble involved in homogeneous nucleation is often H$_2$SO$_4$ (Sassen and Dodd, 1989; Korhonen et al., 1999).

**Implementation of homogeneous nucleation in ICON**

The parameterization of homogeneous nucleation in the microphysics scheme of ICON is based on Kärcher et al. (2006), who also take heterogeneous nucleation into account. The parameterisation of homogeneous nucleation was presented earlier by Kärcher and Lohmann (2002) and has seen minor additions by Ren and Mackenzie (2005).

The center of the calculations is the water saturation ratio over ice $S_i$ (which is essentially an alternative expression to the relative humidity over ice: $\text{RH}_i = S_i \cdot 100$), i.e. its derivative in time:

$$\frac{dS_i}{dt} = a_1 S_i w - (a_2 + a_3 S_i) R_i,$$

with the vertical velocity $w$, a freezing/growth term $R_i$ and the coefficients

$$a_1 = \frac{L_s M_w g}{c_p RT^2} - \frac{M g}{RT},$$

$$a_2 = \frac{1}{n_{\text{sat}}},$$

$$a_3 = \frac{L_s^2 M_w m_w}{c_p p TM},$$

where $L_s$ denotes the latent heat of sublimation of water, $M_w$ the molecular mass of water, $g$ the acceleration of gravity, $c_p$ the specific heat capacity of air, $M$ the mean molecular mass of air, $n_{\text{sat}}$ the number density of water molecules at ice saturation, $m_w$ the mass of a water molecule and $p$ the atmospheric pressure. Equation 8 contains two major processes that determine the change of $S_i$. The first term on the right side of the equation is a production term that increases $S_i$ by vertical motion ($w$ is positive for upward direction) through adiabatic cooling. The freezing/growth term $R_i$ reduces $S_i$ by removing water vapour from the air and adding it to the ice crystals. The full expression of $R_i$ can be found in Kärcher et al. (2006).

In order for homogeneous nucleation to occur, two conditions have to be met first. The ambient temperature $T$ must be lower than -38°C and $S_i$ has to be large enough to reach a critical value $S_{cr}$, which is defined as a function of $T$ in degrees absolute$^{10}$ (Ren and Mackenzie, 2005):

$$S_{cr} = 2.349 - \frac{T}{259}.$$

When rearranging Equation 8 for the freezing/growth term $R_i$, Kärcher et al. (2006) also take into account that pre-existing ice particles lower the ambient water saturation by

$^{10}T$ given in Kelvin but without dimension.
2. DATA AND METHODS

depositional growth. They show that the effect can be displayed in the form of a fictitious downdraft velocity $w_{pre}$ that reduces the effect of the updraft in increasing the saturation. If the critical saturation is met at $S_i = S_{cr}$, and by subtracting $w_{pre}$ from the regular updraft term, Equation 8 results in

$$\frac{a_1 S_{cr}}{a_2 + a_3 S_{cr}} (w - w_{pre}) = R_i.$$  \hspace{1cm} (10)

Therefore, as a last condition for nucleation to occur ($R_i > 0$), it has to be checked, if $w > w_{pre}$, i.e. the increase of $S_i$ as a result of the updraft is larger than the decreasing effect of the pre-existing ice.

If this final condition is met, the scheme proceeds with the calculations for the homogeneous nucleation. The freezing/growth term is calculated according to Kärcher and Seifert (2016), Equation (6), which allows the determination of the number concentration of the ice crystals. After calculating the mean radii of the particles via Equation 23 in Kärcher et al. (2006), the ice water content can be determined geometrically, assuming the particles are spherical. The Fortran code used for this parameterisation can be found in Appendix A.

2.2.4 Model modification

The comparison of the model output with the in-situ data (as will be shown in section 3) implicates that the model does not calculate the homogeneous nucleation correctly. To be reassured that homogeneous nucleation is indeed the underlying process that is too weak and not different processes such as heterogeneous nucleation, the microphysics code is modified in order to increase the likelihood and intensity of the homogeneous nucleation. If with an altered scheme the particle size distribution of cloud ice meets shows good accordance with the in-situ data, the modified parameters are adjusted further to investigate the primary cause of the insufficient nucleation.

There are several parameters that offer themselves to be tuned, some of them only affecting the likelihood of a nucleation event happening, whereas others also increase the strength of their occurrence. Firstly, the critical supersaturation $S_{cr}$, which has to be met for a nucleation event to occur, can be modified by adding a tuning parameter $c_{Si}$ to Equation 9 (see line 34 in Appendix A), which results in a lower critical supersaturation threshold ($mod$ for modified)

$$S_{cr,mod} = 2.349 - \frac{T}{259} - c_{Si}, \quad c_{Si} > 0.$$  \hspace{1cm} (11)

where $c_{Si}$ is a tuning variable that acts as a saturation ratio. For this study three different values for $c_{Si}$ are chosen, which are listed in Table 1. It is important to note that the modification of $S_{cr}$ does not further influence the calculations if a nucleation event occurs.

Additionally, the critical temperature of -38°C could be set to a warmer temperature to
Table 1: Overview of the tuning parameters for the three experiment setups. \(c_{Si}\) reduces the critical saturation ratio \(S_{cr}\), \(w_{TKE}\) increases the strength of the updraft \(w\), and \(c_{pre}\) reduces the strength of the updraft \(w\) by increasing the effect of pre-existing ice particles.

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<tr>
<th></th>
<th>Experiment 1</th>
<th>Experiment 2</th>
<th>Experiment 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c_{Si})</td>
<td>0.3</td>
<td>0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>(w_{TKE})</td>
<td>(0.7 \cdot \sqrt{TKE})</td>
<td>(0.7 \cdot \sqrt{TKE})</td>
<td>(0.7 \cdot \sqrt{TKE})</td>
</tr>
<tr>
<td>(c_{pre})</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

increase the likelihood of a nucleation event. This option is discarded in this analysis since from the results it is clear that the scheme does not produce enough ice particles at temperatures noticeably below -38°C and therefore the temperature threshold most likely is not responsible for this.

Two more mechanisms can be considered, which both, when modified, have an impact on number density and water content of the ice particles once a nucleation event is triggered. One of the mechanisms is the effect that adiabatic cooling has on the saturation ratio and therefore freezing/growth rate by vertical motion \(w\). On the one hand, an increase in \(w\) would increase the likelihood of a nucleation event since the scheme only allows for nucleation to happen if \(w > w_{pre}\) (see line 72 in the code in Appendix A). Moreover, once a nucleation is triggered, the growth rate of the ice particles is enhanced (Equation 10).

Modifying \(w\) has a physical justification as well. Kärcher and Seifert (2016) demonstrate the importance of a good estimate of \(w\) by showing that fluctuations in vertical motion (they use different standard deviations of \(w\)) have a great impact on the distribution of the number density of the newly formed ice crystals. They also argue that climate models yield poor estimates of \(w\) due to a lack of spatial resolution. To compensate for this, the sub-grid variability is included by adding a factor containing the turbulent kinetic energy (TKE) of the model to the grid scale vertical velocity \(w\) (Lohmann et al., 1999; Joos et al., 2008; Köhler, 2013) so that

\[
w_{mod} = w + w_{TKE} = w + 0.7 \cdot \sqrt{TKE}, \tag{12}
\]

where TKE is calculated internally according to Raschendorfer (2001). This expression of \(w_{mod}\) is used in all the experiments in this study except the control run (see line 69 in Appendix A).

Another reason for an insufficient calculation of homogeneous nucleation could be that the effect of pre-existing ice has been modelled to strong. This could be the case if the heterogeneous nucleation parameterization, which was called before, calculated too many or too large ice particles (see Equation 12-13 in Kärcher et al., 2006). To reduce or even eliminate the effect of pre-existing ice, an additional term could be added to modify \(w_{pre}\) so that

\[
w_{pre,mod} = w_{pre} - c_{pre}, \quad 0 \leq c_{pre} \leq w_{pre}. \tag{13}
\]
2. DATA AND METHODS

In the scope of this work, it was not possible to investigate the influence of $w_{pre}$ on the results. All tuning parameters used in this study are listed in Table 1.

2.2.5 Model-to-observation comparison

So far, the observations and the ICON model have only been described in a theoretical manner. In order to obtain a more comprehensive overview of the investigated cloud and the data sets, and to identify possible challenges for the following investigation, a cross section of the frontal cloud for both ICON and the observations is displayed in Figure 3. Figure 3a shows the ICON cloud cover fraction for each grid cell at 11:00 UTC and Figure 3b shows the radar reflectivity for the HAMP radar on board the HALO aircraft. Different variables are displayed for the observation and the model in order to obtain a broader overview and to discourage the reader from comparing the two data sets directly with each other. This is especially relevant for the location of prominent cloud features, since the ICON values are only given for one time step, whereas the HALO measurements were obtained over a time period of a little under half an hour.

![Figure 3](image-url)
However, because of the high spatial resolution of the radar observations, Figure 3b gives an indication on what type of measurements to expect from the in-situ data that was gathered by the FAAM aircraft. The in-situ observations therefore contain information about high ice clouds above and around a height of 8km. In addition, observations incorporate measurements of high water content from a suspected updraft below 4km, since the aircraft passed through a cloud area with large radar reflectivity. The measurements also indicate that the lowest section of the cloud below 2km might well include liquid water.

The investigation of ICON cloud cover fraction does not allow for the identification of individual cloud properties in the same way the radar observations do. However, the distribution of cloud cover does indicate that cloud properties such as number density and water content might be distributed over larger scales than the observations. In addition, the correct placement of small-scale cloud features might be subject to uncertainty e.g. due to the non-linearity of the model. The challenge of this investigation will be to compare the model to the observations despite the differences in resolution and model fluctuations. Thus, the next chapter will present the methods used to prepare the data sets for comparison and show how differences in spatial resolution are accounted for in order to minimize uncertainties as far as possible.

2.3 Methods

2.3.1 Data and model output preparation

Comparing the ICON results to the observations requires some preceding preparation of the model output. The ICON model output first had to be restructured from an unstructured icosahedral-triangular to a rectangular latitude-longitude grid by applying the nearest neighbour method. The remapping was performed via Climate Data Operators (CDO; Schulzweida, 2018).

During the time of the IOP 11, the model output was set to a ten-minute interval to ensure a high comparability to the flight track. For each second of the in-situ measurement time, the ICON values from the grid box that were closest in time, latitude, longitude and altitude were selected, resulting in a 1D-vector dataset that resembled the quasi-height-profile of the measurements. Since this procedure is prone to inaccuracies of the model due to non-linearities or spatial resolution, all quasi-profiles of the neighbouring grid boxes in time or space were also used for comparison. All permutations add up to 81 quasi-profiles.

\[ P = d^4 s^3 = 81 \]

11The expression 'quasi' is used here since the flight track does not follow a constant descent through the cloud.

12The 81 quasi-profiles \( P \) are calculated by permutating the four dimensions \( d \) (time, latitude, longitude and altitude) and 0, 1 or -1 shifts \( s \) (with replacements) which equals \( P = d^4 s^3 = 81 \) permutations (including the case where no dimension is shifted). With dimensions \( d \in [a,b,c,d] \) and shifts \( s \in [0,1,-1] \), the results would be \( \{[a0,b0,c0,d0], [a0,b0,c0,d1], [a0,b0,c1,d1], [a0,b0,c1,d-1], ..., [a1,b1,c1,d1], ..., [a-1,b-1,c-1,d-1]\}.
2. DATA AND METHODS

When showing particle size distributions in the following figures, only those of the 81 quasi-profiles will be shown whose maximum value of their distribution fall into the 5 to 95 percentile range. Showing the neighbouring profiles allows for an estimation of the spatial variability and robustness of the original profile.

The in-situ data are provided with an output frequency of 1 Hz, which when considering the speed of the aircraft \(v_{\text{plane}}\), results in a higher spatial resolution than the average size of the model grid box \(x_{\text{grid}}\). Thus, the in-situ data is temporally averaged over a time interval of \(t_{\text{ave}} = x_{\text{grid}} / v_{\text{plane}}\) to generate better comparability. For an aircraft speed of for example \(v_{\text{plane}} = 150 \text{ ms}^{-1}\) and average grid size of \(x_{\text{grid}} = 2.5 \text{ km}\), the data would be averaged over a period of \(t_{\text{ave}} \approx 17 \text{ s}\).

2.3.2 Calculating the particle size distributions from ICON

The particle size distributions (PSD) from the model are calculated based on the water content \(L\) and the number density \(N\). The calculation follows Seifert and Beheng (2006, Appendix A) and is done for each of the six hydrometeors individually.

The PSDs \(n(m)\) are approximated with modified Gamma functions

\[
n(m) = Am^\nu \exp(-\lambda m^\mu), \quad (14)
\]

with the particle mass \(m\) and the four shape parameters \(A\), \(\nu\), \(\lambda\) and \(\mu\). The parameters \(A\) and \(\lambda\) are dependent on both the water content and the number density:

\[
A = \frac{\mu N}{\Gamma\left(\frac{\nu+1}{\mu}\right)} \left(\frac{\lambda}{\mu}\right)^{\frac{\nu+1}{\mu}} \nu, \quad \text{and} \quad \lambda = \left(\frac{\Gamma\left(\frac{\nu+1}{\mu}\right)}{\Gamma\left(\frac{\nu+2}{\mu}\right) N}\right)^{-\mu}.
\]

The two other parameters \(\nu\) and \(\mu\) are fixed and dependent only on the type of the hydrometeor. They are listed in Table 2.

**Table 2:** Shape parameter \(\nu\) and \(\mu\) and mass-size conversion parameters \(a\) and \(b\) for each hydrometeor.

<table>
<thead>
<tr>
<th></th>
<th>cloud ice</th>
<th>cloud drops</th>
<th>snow</th>
<th>rain</th>
<th>graupel</th>
<th>hail</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\nu)</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\mu)</td>
<td>1/3</td>
<td>1</td>
<td>1/2</td>
<td>1/3</td>
<td>1/3</td>
<td>1/3</td>
</tr>
<tr>
<td>(a)</td>
<td>0.835</td>
<td>0.124</td>
<td>5.13</td>
<td>0.124</td>
<td>0.142</td>
<td>0.1366</td>
</tr>
<tr>
<td>(b)</td>
<td>0.390</td>
<td>1/3</td>
<td>1/2</td>
<td>1/3</td>
<td>0.314</td>
<td>1/3</td>
</tr>
</tbody>
</table>
Since the model calculates mixing ratios for \( L \) and \( N \) (units \([\text{kg kg}^{-1}]\) and \([\text{kg}^{-1}]\)), water content and number density are multiplied with the density of the air. The resulting mass ratios (\([\text{kg m}^{-3}]\) and \([\text{m}^{-3}]\)) can then be inserted into Equation 14.

The PSDs provided by the in-situ measurements are given as a function of the maximum diameter \( D_{\text{max}} \) of the particle. Thus the ICON PSDs are transformed from mass to diameter. Mass \( m \) and diameter \( D \) are connected via empirically determined powerlaw

\[
D = a m^b, \tag{15}
\]

with the two parameters \( a \) and \( b \) that are estimated for each hydrometeor (see Table 2).

To display Equation 14 as a function of diameter instead of mass, the four parameters \( A, \nu, \lambda \) and \( \mu \) are transformed using the expressions given by Petty and Huang (2011):

\[
A_g = \frac{1}{b} A a^{-(1/b)(\nu+1)} \\
\lambda_g = \lambda a^{-\mu/b} \\
\nu_g = \frac{1}{b} (\nu + 1) - 1 \\
\mu_g = \frac{\mu}{b}
\]

By using the parameters \( A_g, \nu_g, \lambda_g \) and \( \mu_g \) the distribution can now be expressed as a function of the particle diameter:

\[
n(D) = A_g D^{\nu_g} \exp(-\lambda_g D^{\mu_g}). \tag{16}
\]

### 2.3.3 Humidity conversions

Relative humidity (RH) is chosen as the main humidity variable in this study as it is closely related to the water saturation ratio \( S_i \), which is the basis of the nucleation scheme. Both measurement data and model output have different humidity variables and must thus first be converted to relative humidity. Conversions from specific humidity to relative humidity were done using the Typhon13 package for Python. The humidity definitions follow Wallace and Hobbs (2006, chapter 3).

The ICON output returns the humidity of the model via specific humidity \( q \). The conversion from specific humidity to relative humidity makes use of the definition the volume mixing ratio VMR. When the VMR is expressed for water vapour, it is defined as the ratio of water vapour pressure \( e \) to the total pressure \( p_{\text{tot}} \)

\[
\text{VMR} = \frac{e}{p_{\text{tot}}}. \tag{17}
\]

The water vapour pressure \( e \) can be expressed using the mass mixing ratio \( x \) (ratio of the

---

13See http://Radiativetransfer.org/misc/typhon/doc/
mass of water vapour to the mass of dry air):

\[ e = \frac{x}{x + \frac{M_w}{M_d}} p_{\text{tot}} = \frac{x}{x + 0.622} p_{\text{tot}}, \]

where \( M_w \) is the molecular mass of water and \( M_d \) the molecular mass of dry air, so that Equation 17 can be rewritten as

\[ \text{VMR} = \frac{x}{x + 0.622}. \]  

Using the definition of the specific humidity \( q \) (ratio of the mass of water vapour to mass of wet air) when reformulated as a function of the mass mixing ratio \( x \)

\[ q = \frac{x}{1 + x}, \]

Equation 18 can now be expressed as a function of the specific humidity:

\[ \text{VMR} = \frac{q}{0.622 (1 - q) + q}. \]  

By using an approximation of the equilibrium vapour pressure of water over ice \( e_{eq,i} \) provided by Murphy and Koop (2005), the relative humidity over ice is given by

\[ \text{RH}_i = \frac{\text{VMR} \cdot p_{\text{tot}}}{e_{eq,i}}. \]  

The humidity variable given by the observational data is the VMR [unit parts per million volume, ppmv]. By multiplying the data with \( 10^6 \) the relative humidity can be calculated via Equation 20.
3 Results and Discussion

This section aims to give an overview of ICON’s two-moment microphysics performance of simulating the frontal cloud during the joint flight context. At first, the calculated water content will be analysed for the cloud profile along the FAAM aircraft flight track. A look at the humidity will then also allow for a first estimation where thermodynamic processes might not be modelled accurately. Thereafter, the number density will be regarded by examining the particle size distributions for different heights. A special focus will be placed on the analysis of the homogeneous nucleation scheme by testing model outputs that were run with different tuning parameters. This is done to understand discrepancies in number densities of small ice particles between the model and measurement data at high altitudes. The chapter will be concluded by testing the scheme’s dependency on the model resolution for accurately modelling homogeneous nucleation.

3.1 Water content and relative humidity

The water content (WC) of the six hydrometeors is one of the two prognostic variables of the microphysics scheme and controls most of the parameterized processes therein. If the WC shows significant disagreement with the measurement data in a certain respect, this will suggest that one or several processes might be insufficiently parameterized. While this study is only a case study, and findings cannot be generalized for the model behaviour in other cases, they may hint at general tendencies the scheme might have.

The WC simulated by ICON is investigated along the FAAM flight track. Figure 4 shows the WC for all six ICON hydrometeors as well as their sum. As a reference, the LWC and IWC measurements from the Nevzorov instrument are also displayed.

The vertical distribution of the WC as shown by the measurement data allows the identification of multiple cloud regimes. At high altitude, the flight route penetrates an area consisting only of frozen particles reaching IWC values of over 0.05 gm$^{-3}$. With decreasing height, both frozen and liquid hydrometeors are present, and the WC reaches a maximum of roughly 0.25 gm$^{-3}$. It is likely that the high WC is a result of a strong updraft located approximately between 2000 m and 4000 m, which is indicated by high radar reflectivity values in Figure 3b, and can also be seen from the retrieved velocities from the Doppler radar based on the Falcon aircraft (no Figure). The majority of the WC in the updraft results from frozen particles, which can be found even below 1000 m, although the ratio of liquid particles to frozen particles increases as expected at lower altitude.

In general, the simulated WC corresponds well to the observations. Throughout the quasi-profile, the simulated WC is in the same order as the measurement data. Smaller offsets can be found in the updraft section, in which ICON overestimates the cloud drop content. At low altitudes, the snow and rain content also exceeds the measurement data noticeably.
At high altitudes, the ice water content seems to match reasonably well, even if the local maximum around 8000 m is simulated at a slightly lower altitude in the model. The height offsets between model and measurement data might have resulted from uncertainties using the nearest neighbour approach, or might simply be model fluctuations or inaccuracies. The overall composition of ICON liquid and frozen hydrometeors seems reasonable, especially when regarding the temperature along the descent (Figure 5b). At approximately 5000 m, the measurement data shows the presence of liquid water, but due to the fact that temperature at that altitude is approximately -20°C with plenty of frozen hydrometeors nearby, the LWC at that height should probably be interpreted with caution and might be a faulty response of the sonde (see section 2.1.3 for details on the Nevzorov probe). However, in general, the simulated WC is found to be sufficiently similar to the measurement data. Differences in LWC in the updraft section and overall WC in the lower altitudes are not large enough to imply that the scheme is incorrect but instead might well be a result of random fluctuations or model inaccuracy. Thus, these differences will not be further investigated in this study.

A further step in examining the cloud physics is by looking at the relative humidity (RH).
Values of RH for both the model output and observations are displayed in Figure 5a. The

![Figure 5: Quasi-profiles for relative humidity (a) and temperature (b) along the FAAM flight track. ICON values are given in blue and measurement data in orange. The vertical axis is the same as in Figure 4.](image)

measurement data indicates that for the majority of the descent between 8000 m and 2000 m, the humidity takes on values around the saturation mark of 100% RH with a deviation of roughly 10-15 percentage points\(^\text{14}\). Above 8000 m, the RH rapidly decreases in the observations even though the presence of IWC is measured until 8300 m. For values below 8000 m, the model output follows the measurement profile but shows significantly less deviation. The ICON profile is considerably less smooth, especially for the temperature. This is simply a result of the choice of grid boxes along the profile. Since the vertical axis is constant in time, and for each second of the observations the value of the corresponding grid box is taken, the resulting ICON profile shows an incremental behavior due to the lower spatial resolution (c.f. Section 2.3.1). Above 8000 m, ICON’s RH noticeably exceeds the measurement data and only decreases above 8300 m. In addition, ICON shows values of nearly 125% RH, which are the highest values throughout the profile. Presumably the high humidity is the result of insufficient nucleation and vapour deposition onto the particles.

\(^{14}\)For the calculation of the entire profile, the RH was calculated by using the water saturation ratio over ice. Effects due to the presence of a liquid phase were not taken into account and may have slightly distorted the results at altitudes where liquid water was present.
3. RESULTS AND DISCUSSION

At temperatures around -40°C, the physically dominant process responsible for creating hydrometeors and removing water vapour from the atmosphere is homogeneous nucleation. This finding is further explored in the following chapter when analysing the particle size distributions.

3.2 Particle size distributions

An accurate representation of the particle size distribution (PSD) is important for a variety of cases such as the growth of precipitation, cloud modelling and radar meteorology (e.g. Houze et al., 1979) and there have been several attempts to parameterize the PSDs (e.g. McFarquhar and Heymsfield, 1997; Field et al., 2007). The parameterization of the PSD used here by Seifert and Beheng (2006) is based on both moments $N$ and $L$ (Eq. 2 and 3).

As a reference for the ICON PSD, the PSD measured by the FAAM aircraft is used and displayed in Figure 6. The PSD as determined by the measurement data contains measurements from three individual instruments that are complementary in size range detection. For drop sizes roughly over 50 µm, the measured distribution shows comparably little standard deviation (CIP-15 and CIP-100 measurements). Measurements for smaller particles covered by the CDP instrument have higher deviation, and values should therefore be considered with caution. Nevertheless, at most heights the observations show a gamma-like distribution, even if the tail at the smaller side is more uncertain. With decreasing height, the distribution shows a tendency for large particles to increase in size and the transition from large to small particles to be less steep than at higher altitudes. If the CDP measurements are to be trusted, the highest number density within the cloud is found at low altitudes for particle sizes around 10 µm. Since the temperature is around the freezing point and there is a presence of snow (large particles), the small particles are presumably liquid cloud drops, since a presence of liquid hydrometeors is indicated in Figure 4. At high altitudes the distribution looks more gamma-like, with the difference that the maximum particle diameter is smaller than 1000 µm and number densities rapidly increase with decreasing size. For very small particles with smaller diameter than 10 µm, the measurements show a decrease in density, but this finding is coupled with high uncertainty. All particles at high altitude, as indicated by low temperatures and distribution of LWC and IWC in Figure 4, are most likely frozen.

For comparison with ICON, the measurements from Figure 6 are used but for simplicity henceforth displayed without the standard deviation. Figure 7 shows the PSD for each of the six hydrometeors against the measurements data. To get a feeling for the spatial variability, and to account for possible mismatches between measurements and ICON profile, PSDs from the neighbouring grid boxes (showing the distributions with 5-95% of the maximum value) are also displayed. Throughout the height levels, ICON shows good agreement with the measurement data concerning the large particles. In most cases, even the transition to
Figure 6: Number densities as a function of maximum diameter of a particle for the three instruments CDP (orange points), CIP-15 (blue points) and CIP-100 (green points). The shaded area marks the standard deviation of the measurement for the displayed height. Height intervals of 1000 m are shown from top left to bottom right, covering an altitude from 1000 m to 9000 m. The temperature is the mean measured temperature in the height interval.
3. RESULTS AND DISCUSSION

Figure 7: Particle size distributions for the six ICON hydrometeors Ice (red), Cloud drops (grey), Snow (yellow), Rain (purple), Graupel (light green) and Hail (pink). The sum of the hydrometeors is indicated by the dotted line. Paler lines show PSDs for surrounding grid boxes within the 5-95 percentile range for the equivalent hydrometeor. Orange, blue and dark green points show the measurement data as shown in Figure 6. Axis and mean temperature are also the same as in Figure 6.
smaller particles is in accordance with the data. At low altitudes, cloud drops dominate
the spectra of small particles, exceeding number densities for the measurement data, but
are possibly within the margin of uncertainty. All particles above 3000 m are frozen with a
higher proportion of ice particles than snow particles. At altitudes where no cloud drops
are simulated, significantly fewer small particles (ice and snow) are simulated than the
measurements indicate, even taking the high uncertainty of the measurements into account.
This behaviour is especially prominent above 7000 m, where measurement data show a
gamma-like behaviour. At temperatures below -38°C, homogeneous nucleation is the
physically dominant process that produces ice particles (see chapter 2.2.3). At most heights
the PSDs of the neighbouring grid boxes also show a similar behaviour to the main profile,
with the exception of the 7000 m-8000 m interval, in which the PSDs spread significantly
towards higher number densities. This is a possible indication that homogeneous nucleation
might have occurred in neighbouring grid boxes, especially around the -38°C threshold.
At higher altitudes, the model shows a robust tendency to underestimate particle number
densities. Combined with the result from chapter 3.1, which showed that at this height,
there was an overestimation of relative humidity, it is reasonable to assume that ICON
struggles with the accurate representation of homogeneous nucleation for this cloud. To test
this assumption and investigate further causes for this, the ICON scheme for homogeneous
nucleation is modified and the output compared to the control simulation in the following
chapter.

3.3 Sensitivity studies on homogeneous nucleation

The assumption is tested that the deficiencies in representing small particles and relative
humidity at high altitudes are a result of an insufficient parameterization of homogeneous
nucleation by the microphysics scheme. Therefore, the two following questions are addressed
and investigated:

- If homogeneous nucleation is the dominant effect for not modelling enough (small) ice
  particles, can an accurate representation be forced by adjusting the scheme?
- And if it can be forced, what factors cause the scheme to underestimate homogeneous
  nucleation?

Forcing homogeneous nucleation

For the first question, it is assumed that the nucleation scheme was not activated at all (or
at least in most grid boxes along the flight track) and the ice displayed at altitudes above
7000 m is pre-existing ice not produced by the scheme. In this case, the simple activation of
the scheme would provide sufficient ice particles without any modification of the nucleation
intensity needed. To test this assumption, the humidity threshold, which has to be exceeded
for a nucleation event to occur, is reduced. According to Equation 9, the humidity threshold $S_{cr}$ ranges from 1.44 (144% RH) at -38°C to 1.47 (147% RH) at -44.5°C, which was the lowest measured temperature during the descent. With respect to the humidity simulated in the unmodified simulation (which from now on will be referred to as the 'control' simulation, Figure 5), the threshold is reduced by 0.1, 0.2 and 0.3. A reduction of 0.3 results in a new humidity threshold of 1.14 to 1.17 (114% to 117% RH), which should be exceeded in most if not all grid boxes with assumed homogeneous nucleation. The reduction by 0.1 and 0.2 shall give an insight into whether and to what extent homogeneous nucleation might occur at lower threshold reductions.

In addition to modifications to the $S_{cr}$ threshold, the vertical velocity that is used by the scheme is increased by adding a scaling factor that is dependent on the turbulent kinetic energy of the model. The same scaling factor is used throughout all of the three threshold reduction experiments. This approach is legitimate in order to take into account sub-grid scale variability (see chapter 2.2.4).

The further analysis will now only focus on the altitude range above 7100 m since below that height, temperatures within the ICON levels are too high to allow for homogeneous nucleation. Height intervals of 300 m are chosen as each interval contains one ICON height level. Figure 8 shows the PSDs of the control simulation as in Figure 7, but at higher resolution for only high altitudes. Temperatures above 7100 m range from 300 m mean values of -34°C to -43°C. Assuming the temperature mostly deviates around 3 K at each interval, these settings allow for an inspection of the transition from heterogeneous to homogeneous nucleation between 7400 m and 7700 m. At this interval, both nucleation types are possible, whereas below only heterogeneous nucleation occurs.

At the lowest height interval, the PSD only slightly underestimates the number density. However, taking the neighbouring PSDs into account, the difference is not especially large and may result from spatial variability. The two higher height intervals until 8000 km also show a large spread in neighbouring PSDs but consistently underestimate the measurement data, which implies that the underestimation is a result of the model and not the selection of the grid points on the flight profile or a computational spatial 'mismatch'. In the region where homogeneous nucleation is expected, the PSDs show consistent behaviour with height. The comparably low spatial variability of in the uppermost height interval compared to the lower ones may be a result of the chosen flight track of the aircraft, which did not descend evenly but instead spent roughly the same amount of time between 8000 m - 8300 m as it did for the descent from 8000 m - 7000 m (see also Figure 3). Therefore, outliers may have been reduced in their impact by averaging over a larger number of grid boxes.

The next step of the experiment is to test whether a correct representation of homogeneous nucleation can be forced by adjusting the model settings. Therefore, the first look will be at the 'physically strongest' modification of reducing the humidity threshold by 0.3 (see 'experiment 1' in Table 1 for an overview of the tuning parameters). Figure 9 shows the
results from the modified model setup. Throughout all height levels, the model now shows far closer agreement to the measurement data. Especially the number densities of ice in the regions where homogeneous nucleation is suspected has increased significantly compared to the control run. Although there is still a noticeable spatial variability, the results indicate that the modified settings have successfully triggered the homogeneous nucleation scheme. The increase of small particles has seemingly occurred at the cost of larger particles, which would have been the direct result of more small ice particles competing with the pre-existing ice and snow particles for the available humidity.

With the addition of the TKE scaling factor for vertical velocity, the results show sufficient
agreement with the measurement data such that it can be assumed that either one of the tuned parameters or both are responsible for the misrepresentation of the scheme. From this experiment alone it is still unclear whether the intensity of the event was misrepresented in the control run or if the event simply did not occur at all. However, the analysis of the other experiments will suggest that the reason for the misrepresentation it is the latter.

Thus, if the ICON microphysics scheme is able to appropriately simulate homogeneous nucleation at a strong threshold reduction of 0.3, is it possible to also do so at a lower threshold reduction, and if so, by how much?

To answer this question, simulations with $S_{cr}$ reductions of 0.2 and 0.1 (see ‘experiment 2’ and ‘experiment 3’ in Table 1 for an overview of the tuning parameters) were evaluated.
Figure 10 shows the PSDs at high altitude for the 0.2 humidity threshold reduction setup ('experiment 2'). Compared to experiment 1, the results show a decrease in number density for smaller particles at all heights. This is especially noticeable for the 7400 m to 8000 m height region. It is noteworthy that the PSDs at height interval 7400 m to 7700 m show very little spatial variability although at this altitude, heterogeneous nucleation is at least partly possible. Furthermore, at the topmost altitude, there is a small decrease in number density. There is however a slight increase in larger particles. This leads to the assumption that a reduction of 0.2 in humidity threshold is not enough to ensure that the results are as similar to the observations as in experiment 1. Although the PSDs have still noticeably improved in the representation of small particles compared to the control simulation, the differences to the results in experiment 1 indicate that homogeneous nucleation has only occurred in an...
3. RESULTS AND DISCUSSION

insufficient number of grid boxes. This theory is supported by the fact that the strength of the nucleation has not been changed by the tuning parameters compared to experiment 1. Of the two modified parameter, only the modification of the vertical velocity can impact the strength of the nucleation. However, the same vertical velocity tuning term was used for all experiments apart from the control run.

To close the gap from experiments 1 and 2 to the control simulation, the last experiment ('experiment 3') is regarded, that contains a reduction in the humidity threshold by 0.1. The PSDs from this experiment are shown in Figure 11. As expected, the PSDs in experiment 3 are consistently lower than those in experiment 2. This supports the hypothesis that homogeneous nucleation is triggered in fewer grid boxes for a lower humidity threshold.

![Figure 11](image-url)

**Figure 11:** Particle size distributions for the modified experiment setup with the humidity threshold \( S_{cr} \) reduced by 0.1 and the vertical velocity \( w \) scaled with \( w \cdot TKE \). Figure axis, measurement data, mean temperature and line colors are the same as in Figure 8.
reduction and is not caused by a variation in the strength of the nucleation event. This is also visible in the slight tendency of the PSDs towards larger particles. Interestingly, the PSDs for the height intervals from 7100 m to 7700 m have reduced in number density for smaller particles compared to the control simulation. This is possibly the result of less heterogeneous nucleation since homogeneous nucleation must have occurred in some grid boxes. Both nucleation processes rival for the available humidity, but the causes of this could also lie in more complex interactions of particles between the height intervals (e.g. less heavy particles falling into the lower altitude level due to a lack of growth because of increased homogeneous nucleation). However, taking into account the spatial variability of the PSDs in the lower altitudes, this difference might also be insignificant.

Summarizing the three experiments, only reducing the humidity threshold by 0.3 results in PSDs that are sufficiently similar to the measurements. For both of the other experiments (reduction by 0.2 and 0.1), the number density of the small ice particles reduces compared to a higher threshold reduction and corresponds less well to the measurement data. Although reducing the humidity threshold does not have an influence on the strength of the nucleation but instead on the likelihood of an event happening, each increase in threshold reduction shows an increase in number density of small particles and also results in a reduction of ambient relative humidity (Figure 12). The modification of the vertical velocity $w_{\text{mod}}$ with the TKE is the only setting changed which has an impact on the intensity of the nucleation. Nonetheless, the expression for $w_{\text{mod}}$ is the same for all experiments (excluding the control

Figure 12: Quasi profiles for relative humidity along the flight track for the control in (a), experiment 3 (b, $S_{cr}$ threshold reduction by 0.3), experiment 2 (c, $S_{cr}$ threshold reduction by 0.2) and experiment 1 (d, $S_{cr}$ threshold reduction by 0.1). ICON values are given in blue and measurement data in orange. Vertical axis as in Figure 4.
run), and values only differ if grid scale vertical velocity or TKE change as a result of the different behaviour of the homogeneous nucleation scheme. Therefore, with the exception of the control run where \(w\) has not been modified, changes in \(w_{mod}\) values throughout the experiments are considered insignificant.

This leads to the assumption, that an incremental decrease in small particles for the experiments is likely a result of a decreased number of grid boxes that allow homogeneous nucleation. For each height level, several grid boxes are averaged. If, for each of the humidity threshold reductions, more individual grid boxes meet the requirements for nucleation, the progressive difference in PSDs could easily be explained by the averaging.

**Investigating the dependence on model resolution**

From the previous experiments on threshold reduction, it appears as if some grid boxes do not allow for homogeneous nucleation because the humidity is too low to meet the threshold value, although measurements indicate that they should. The calculation formula for the humidity threshold (Eq. 9) is an analytical fit to measurement data from Koop et al. (2000), and high threshold values are assumed to be physically meaningful.

Thus, why does the model simulate (significantly) less humidity than necessary for the nucleation scheme to be triggered, when the measurement data suggests it to be the case? The reason for this may, to a great extent, lie in the coarse resolution of the model and its inability to sufficiently display small scale fluctuations of humidity.

It is known that fluctuations of water vapour have a substantial effect on the number of newly formed ice particles (Easter and Peters, 1994). The effect of small-scale vertical velocity fluctuations on the distribution of newly formed ice particles is also known to be important (e.g. Kärcher and Ström, 2003; Kärcher and Seifert, 2016), and is allowed for in all experiments by scaling the vertical velocity with the TKE. However, turbulence fluctuations are not taken into account in the scheme, although its impact may be important as well. It is assumed here that the scale at which homogeneous nucleation occurs, is smaller than the average grid size used for the work here, which is 2.5 km horizontally. If a hypothetically small area, e.g. an area the size of half a grid cell, had a humidity large enough to meet the threshold (by fluctuation, upward motion or simply a stochastic event), then nucleation would occur. If the grid box that represented that area because of its large size also covered an other area, that was drier, the result might be that the humidity averaged over the entire grid box is too low for the threshold to be met. In this case, the scheme for the grid box would not allow for homogeneous nucleation at all, instead of partial nucleation, which would lead the results to be more similar to the measurement data.

If the theory that the model resolution is too coarse to allow for sufficient nucleation is correct, then ideally a model at very fine resolution (e.g. an LES simulation) would simulate
homogeneous nucleation accurately without threshold reduction (and possibly $w$ modification) being necessary. Simulating ICON in LES mode for a fine resolution was not possible during the scope of the analysis, but the original ICON simulation of 2.5 km resolution was set up to have a nested model with approximately half the grid size of 1.25 km. However, a reduction of the grid size by factor 2 will most likely not allow for sufficient homogeneous nucleation with the control simulation. Nonetheless, the finer grid may allow for more grid boxes to enable nucleation at lower threshold reductions.

At first, the PSDs of the control run for both resolutions are compared in order to see whether a finer resolution causes any noticeable changes without any modifications. Figure 13 shows the PSDs for heights above 7100 km as in Figure 8 but in comparison to the PSDs for the higher resolution nest. As expected, for the control simulation, the finer grid resolution does not have a substantial impact on the PSDs. If at all, the coarser resolution run simulates more small particles at the lowest, non-homogeneous nucleation permitting altitude. The finer grid simulations show less spatial variability for the lower height levels, but this may well be the result of the neighbouring grid cells being spatially closer than in the coarser model. At the highest altitude some neighbouring grid boxes show that the PSDs shift towards smaller particles, but the finer resolution also allows for higher likelihood in spatial miss-matches than the coarser.

Although for most of the regarded heights in experiments 1-3, PSDs for both resolutions show very similar behaviour, there is a substantial difference in experiment 2. Figure 14 shows the PSDs for experiment 2 (humidity threshold reduction by 0.2) for both resolutions (comparisons of the PSDs for experiment 1 and 3 are shown in Figure B.1 and B.2 in Appendix B). While in this experiment, the coarser grid simulation does not show a high number density for the small particles and is comparable to the control run, the finer grid simulation at 7400 m to 8000 m shows a significant increase in small particles. This is a strong indication, that the sub-grid variability of humidity is the main driver for the scheme to underestimate homogeneous nucleation. By regarding the spatial variability, it seems as if the combination of threshold reduction by 0.2 and resolution reduction to 1.25 km was a ‘lucky’ combination to trigger homogeneous nucleation during the flight profile, while most neighbour profiles had not (yet) been triggered. Nevertheless, this example does serve as a strong indication that the underestimation of homogeneous nucleation is largely due to the model’s inability to sufficiently display humidity fluctuations.

The results so far all indicate that the models inability to sufficiently display homogeneous nucleation is due to the coarse model resolution and the inability to account for smaller scale humidity fluctuations. Although this is the most obvious cause, and the movement towards higher resolution models is motivated by the prospect of small-scale effects being calculated directly, other effects might also be important. In this study the effect of heterogeneous nucleation at temperatures lower than -38 °C is not considered. However, heterogeneous ice nuclei that are thermodynamically not able to reduce the energy barrier sufficiently also
Figure 13: Particle size distributions for the control run for the large domain with 2.5 km resolution (top row) and for the nest with 1.2 km (bottom row). Figure axis, measurement data, mean temperature, line colors and height intervals as in Figure 8.
Figure 14: As Figure 13, but for experiment 2 (humidity threshold $S_{cr}$ reduced by 0.2).
3. RESULTS AND DISCUSSION

depending on aerosol concentration play a more or less dominant role (Gierens, 2003; Kärcher and Lohmann, 2003). Interactions between the nucleation and growth rate of heterogeneous and homogeneous nuclei might be important but are also not considered here. Moreover, the effect of pre-existing ice is not further regarded than its original implementation in the scheme (Eq. 10). An increase of $w$ by scaling with the TKE may have reduced the impact of pre-existing ice significantly. Another factor of uncertainty may be, as already stressed in section 2.3.1, the choice of analysed grid boxes via nearest neighbour method. Although regarding the profiles of the neighbouring grid boxes does indicate the spatial variability, the 'correct' grid box (i.e. the grid box that is supposed to simulate the microphysics at the aircraft measurement location) cannot be determined with certainty. Finally, as in all sensitivity studies, output results are subject to uncertainties and fluctuations due to the nonlinear nature of the model.
4 Summary and Conclusions

In this study, the main cloud microphysical parameters of the ICON two-moment scheme (Seifert and Beheng, 2006) properties were investigated for a case study of a frontal cloud. Airborne in-situ measurements taken during the NAWDEX joint flight on 14 October 2016 are used to evaluate the model output. This allows for an examination of several different cloud regimes since measurements are available in a quasi-profile from the cloud top to the cloud base. The fact that the microphysics scheme calculates two prognostic variables for each hydrometeor class allows for a differentiated analysis of both water content and particle size distribution. ICON output and measurement data are compared by selecting grid points in time and space that have the closest accordance with the aircraft location. This method is sensitive to errors resulting from model inaccuracies and coarse resolution but these are restricted by also regarding the quasi-profiles of the spatially and temporally neighbouring grid cells. ICON is set to run at a spatial resolution of roughly 2.5 km but also contains a one-way nest at double the resolution.

As a first step towards analysing the microphysics scheme, the distribution of water content throughout the cloud was evaluated. The measurement data allowed the identification of several different cloud regimes, mostly subject to altitude. At the cloud base, water content is comparably low and liquid and ice water are found in roughly same proportions. Moreover, the data shows a region with high ice water content, presumably an updraft section. Towards the cloud top the properties shift more towards a pure ice cloud that reaches over 8 km altitude. ICON was able to represent the distribution of water content reasonably well. Most of the differences in water content throughout the quasi-profile can be disregarded as the order of magnitude mostly is the same. Noticeable albeit not too large differences could only be found in the updraft region, where ICON calculates too much liquid water compared to the measurements and in the lowest region, where too much snow and rain is simulated.

Following the analysis of the water content, the relative humidity of the quasi-profile was evaluated to indicate whether the right amount of water is deposited onto the surrounding hydrometeors. The measurement data shows that spatial variability in humidity deviates roughly 10 to 15 percentage points around the mean profile values, whereas ICON shows a much weaker behaviour. In addition, ICON’s mean RH profile is in accordance with the mean RH profile of the measurement until 8 km height but shows a significant increase above whereas the measurement data show a strong decrease. This finding is an indication of insufficient representation of homogeneous nucleation in the model.

Exploiting the fact that the number density of the particles is explicitly calculated in the Seifert and Beheng (2006) scheme, the PSDs for all hydrometeors are compared to the measurement data. At first the robustness of the measurement PSDs is tested by considering the standard deviation that arises by averaging the data for 1 km height intervals. The size distribution obtained by the observations is highly robust for particles larger than
50 µm as the measurement devices responsible for detecting larger particles are more precise. Measurements for particles smaller than 50 µm are more uncertain and a direct comparison with the model output is thus to be considered with caution.

The ICON PSDs were evaluated for eight height intervals between cloud base and cloud top. At low altitudes, ICON simulates the distribution of large particles well, assuming rain, ice and snow particles to be the main large hydrometeors. The distribution of small particles at low heights is likely to be overestimated by ICON cloud drops, but this cannot be claimed with certainty due to the high standard deviation of the measurement. For center and top of the cloud, ICON represents large particles well with a combination of ice and snow particles. With the absence of cloud drops above 3 km, ICON generally underestimates the number of small particles. Just like the RH overestimation at the cloud top, the lack of small particle production is most likely also the result of an insufficient representation of homogeneous nucleation in the model. In general, homogeneous nucleation is assumed to be the main driver of particle production at that altitude (for temperatures below -38°C).

In order to analyse the deficient behaviour of the parameterization, two parameters within the homogeneous nucleation scheme in ICON were modified in order to increase the likelihood of homogeneous nucleation events and their strength. The likelihood of nucleation occurrence was increased by incrementally reducing the humidity threshold (reductions of 0.1, 0.2 and 0.3) necessary for the parameterization to be 'switched on'. The strength of the nucleation event was increased by adding a tuning term to the vertical velocity in the scheme that correlates to the model turbulent kinetic energy and thus accounts for small-scale velocity fluctuations. Analysing the PSDs for heights over 7 km shows that for a drastic threshold reduction of 0.3, ICON is able to display the size distribution well compared to the measurement data even if at the cost of slightly underestimating the large particles. The conclusion is that the scheme is able to sufficiently simulate a distribution where homogeneous nucleation occurs, but under un-physically low values of the humidity threshold. Along this experiment, two less extreme threshold reductions were considered.

Reducing the threshold by 0.2 shows lower numbers of small particles compared to the first experiment, from which it is implied that the scheme already underestimated the nucleation even though the threshold is reduced significantly. The third experiment of threshold reduction of 0.1 shows a further reduction of small particles. Since the strength of the homogeneous nucleation event was not changed, the progressive increase of small particle production at a lower threshold is most likely subject to the small-scale nature of the nucleation event. The humidity threshold itself is not too high as it has been validated by measurements. Thus, the high humidity values possibly occur on mostly small scales, so that averaged humidity values calculated in a grid box would tend to fail to reach the threshold value, even if within the area nucleation could physically occur.

To test this theory, the higher resolution model nest was regarded to investigate differences in nucleation behaviour resulting from change in resolution. Comparisons of size distributions
at high altitude for both resolutions in the control simulation show a very similar behaviour. Although for experiment 1 and 3, the PSDs were also found to be similar for both resolutions, support for the hypothesis was found in the evaluation of experiment 2. Compared to the low resolution, the high resolution nest simulates significantly more small particles between 7.4 km and 8 km, where homogeneous nucleation is suspected of playing an important (or for the most part dominant) role. Examining the surrounding profiles shows that not all PSDs increase to the same extent but still show a tendency to increase the number of small particles. Nonetheless, this case supports the idea that homogeneous nucleation happens on sub-grid scales and a finer model resolution would allow for homogeneous nucleation to happen with settings that are closer to physically meaningful ones. As a conclusion, this study suggests that at the current model resolution of 2.5 km, the humidity saturation threshold given in Eq. 9 is most likely the limiting variable that prohibits ICON from displaying homogeneous nucleation the closest to reality.

Although this work shows support for this hypothesis in two ways, by testing the influence of different humidity threshold settings and the model resolution on the size distribution, the possibility of additional factors also contributing to particle distribution cannot be disregarded. It was assumed that all cloud nuclei that trigger heterogeneous nucleation do so at higher temperatures than -38 °C, below which homogeneous nucleation becomes possible. Although for most ice nuclei, this might be the case, other studies have found less potent ice nuclei to nucleate at similar temperatures to homogeneous nucleation. In addition, the influence of pre-existing ice was also not investigated in this study and may have an important influence on both the likelihood of nucleation occurrence of the scheme as well as intensity. Finally, it must to be emphasised that due to the single-line measurement to model comparison, errors and uncertainties due to lead-lag errors or coarse model resolution cannot be eliminated, even if the evaluation of the neighbouring grid boxes helps to account for this. To test and possibly verify the hypothesis, further research is necessary.

**Outlook**

This work has suggested that the sufficient representation of homogeneous nucleation in ICON is sensitive to model resolution and that the output improves with finer resolution as a result of better display of humidity fluctuations. This hypothesis can be tested in two ways. Firstly, other factors possibly influencing the nucleation at high altitudes have to be regarded in order to quantify their effect. A possibility would be to reduce or eliminate the effect of pre-existing ice on homogeneous nucleation. This could be done by modifying $w_{pre}$ in Eq. 10. By keeping the settings as in experiment 3, where adequate homogeneous nucleation is assumed, the effect of pre-existing ice on ice production could be investigated. This study has also chosen not to untangle the effect of the modified velocity parameter from the humidity threshold modifications in the three different experiments due to its limited scop.
4. SUMMARY AND CONCLUSIONS

If experiment 3 is able to force an accurate representation of homogeneous nucleation in a sufficient number of grid boxes, does the vertical velocity still have to be increased for the intensity to be similar to the measurements?

The great uncertainty of the model-to-flight track comparison is difficult to meet if only these two data sets are considered due to the one-dimensionality of the aircraft data. In addition to investigating the effect in different in-situ measurements, an easier option would be to include measurements that cover greater areas for example by considering passive or active remote sensing data. The 'joint flight’ offers the possibility of looking into radar or radiometer data if they offer a sufficiently high resolution view of the cloud tops and could also be combined with an evaluation of humidity measurements obtained by several dropsondes.

The second, more direct, approach to testing the hypothesis would be running the model at several different resolutions. If the hypothesis were correct, it would be expected that from a sufficiently high resolution onward, the model would simulate fluctuations in humidity and velocity directly resulting in an accurate simulation of homogeneous nucleation without model adjustments. This would give a further insight into the scale of the fluctuations and nucleation events as one could track the change of the effect for decreasing grid sizes. Although an increased model resolution brings its own challenges, such as the increased difficulty of matching measurement data and model output as well as a higher chance of fluctuations being misplaced or chaotically distributed, this approach combined with careful uncertainty analysis offers the chance to quantify the effect and verify or falsify the hypothesis.
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In memory of

Verena Grützun, who supervised and mentored me for both my Bachelor and Master thesis.
References


Appendix A  Implementation of homogeneous nucleation in ICON

The following code calculates number density, water content and the resulting atmospheric humidity for each hydrometeor in a homogeneous nucleation event. The code owner is Axel Seifert. Modifications were implemented by Aiko Voigt. The code has been slightly altered for better comprehensibility. Variables such as constants are defined elsewhere in the code and are mentioned by use of a placeholder. The function for heterogeneous nucleation has also been replaced by a placeholder.

```fortran
SUBROUTINE ice_nucleation_homhet
  !**********************************************************************
  ! Homogeneous and heterogeneous ice nucleation
  ! Nucleation scheme is based on the papers:
  ! - Kaercher and U. Lohmann, 2002 (KL02 hereafter)
  ! - B. Kaercher, J. Hendricks and U. Lohmann 2006 (KHL06 hereafter)
  ! with additions by C. Ren and A.R. Mackenzie 2005 (RM05 hereafter)
  ! implementation by Carmen Koehler and Axel Seifert
  !**********************************************************************

  ! PLACEHOLDER FOR VARIABLE DECLARATION

  !**********************************************************************
  ! PLACEHOLDER FOR HETEROGENEOUS NUCLEATION FUNCTION
  !**********************************************************************

  ! Begin homogeneous nucleation calculation using KHL06 approach
  ! Begin homogeneous nucleation calculation using KHL06 approach
  DO k = kstart, kend
    DO i = istart, iend
      ! loading atm. pressure, temperature and saturation, calc. saturation ratio
      p_a = atmo%p(i,k)
      T_a = atmo%T(i,k)
      e_si = e_es(T_a)
      ssi = atmo%qv(i,k) * R_d * T_a / e_si

      ! critical supersaturation for homogeneous nucleation (RM05)
      ! and additional tuning constant c_hom_ssi
      scr = 2.349 - T_a * (1.0_wp/259.00_wp) - c_hom_ssi

      ! check if critical saturation and temperature are reached
      IF ( ssi > scr .AND. T_a < 235.0 .AND. ice%n(i,k) < ni_hom_max ) THEN
        ! load and calculate parameters for preexisting ice (-> w_pre)
        n_i = ice%n(i,k)
        q_i = ice%q(i,k)
        x_i = particle_meanmass(ice, q_i,n_i)
        r_i = (x_i/(4./3.*pi*rho_ice))**(1./3.)
      ENDIF
    END DO
  END DO
```


v_th = \text{SQRT}\left(8.0 \times k_b \times T_a/(\pi \times m_a)\right)

\text{flux} = \alpha_d \times v_th/4.

n_sat = e_{si} / (k_b \times T_a)

! coefs of supersaturation equation
acoeff(1) = (L_{ed} \times \text{grav}) / (cp \times R_d \times T_a^{**2} - \text{grav}/(R_l \times T_a))
acoeff(2) = 1.0/n_sat
acoeff(3) = (L_{ed}^{**2} \times M_w \times m_w)/(cp \times p_a \times T_a \times M_a)

! coefs of deposition growth equation
bcoeff(1) = \text{flux} \times svol \times n_sat \times (s_{si} - 1.)

bcoeff(2) = \text{flux} / \text{diffusivity}(T_a,p_a)

! pre-existing ice crystals included as reduced updraft speed
ri_dot = bcoeff(1) / (1. + bcoeff(2) \times ri)

! Eq. 12 KHL06 freezing/growth term for preexisting ice
R_{ik} = (4 * pi) / svol * n_i * r_i^{**2} * ri_dot

! KHL06 Eq. 19 calculate fictional downdraft as effect of preexisting ice
w_pre = (acoeff(2) + acoeff(3) \times s_{si}) / (acoeff(1) \times s_{si}) \times R_{ik}
w_pre = \text{MAX}(w_pre,0.0_{wp})

! load (and calculate) vertical velocity
\text{w_hom} = c_{hom_w} \times \text{atmo\%w}(i,k+1) + c_{hom_tke} \times \text{sqrt}(\text{atmo\%tke}(i,k+1))

! check if updraft effect > preexisting ice effect
IF (\text{w_hom} > \text{w_pre}) \text{THEN} ! homogenous nucleation event

! timescales of freezing event (see KL02, RM05, KHL06)
! Eq. 16 KHL cooling be adiabatic rising
cool = \text{grav} / cp \times w_hom
ctau = T_a * (0.004 * T_a - 2.0) + 304.4

! freezing timescale, eq. (5)
tau = 1.0 / (ctau \times cool)

! dimensionless aerosol radius, eq. (4)
delta = (bcoeff(2) \times r_0)

! left side of Eq. 14 or 21 KHL06
\phi = acoeff(1) \times s_{si} / (acoeff(2) + acoeff(3) \times s_{si}) / (w_hom - \text{w_pre})

! monodisperse approximation following KHL06
! kappa, Eq. 8 KHL06
kappa = 2.0 * bcoeff(1) * bcoeff(2) * tau / (1.0 + delta)**2

! root of kappa
sqrtkap = \text{SQRT}(kappa)

! analytic approx. of \text{erfc} by RM05 (Eq. 24) -> KHL06 (Eq. 7) \ f(kappa)
ren = 3.0 * sqrtkap / (2.0 + \text{SQRT}(1.0 + 9.0 * kappa/pi))

! first part of Eq. 6 KHL06
R_{imfc} = 4.0 * pi * bcoeff(1) / bcoeff(2)**2 / svol

! Freezing rate RIM for given radius Eq. 6 KHL06
R_{im} = R_{imfc} / (1.0 + delta) * (delta**2 - 1.0 &
& + (1.0 + 0.5 * kappa * (1.0 + delta)**2) * ren/sqrtkap)

! number concentration and radius of ice particles
! ni Eq.9 KHL06
ni_hom = \phi / R_{im}

! for Eq. 3 KHL06
ri_0 = 1.0 + 0.5 * sqrtkap * ren

! mean particle radius, Eq. 3 KHL06 * REN = Eq.23 KHL06
ri_hom = (ri_0 * (1. + delta) - 1.) / bcoeff(2)

! Water content calculation assuming spherical particles
mi_hom = (4./3. * pi * rho_ice) * ni_hom * ri_hom**3
mi_hom = MAX(mi_hom, ice%x_min)

nuc_n = MAX(MIN(ni_hom, ni_hom_max), 0.0_wp)
nuc_q = MIN(nuc_n * mi_hom, atmo%qv(i,k))

! Return new values for number density, ice water content and humidity
ice%n(i,k) = ice%n(i,k) + nuc_n
ice%q(i,k) = ice%q(i,k) + nuc_q
atmo%qv(i,k) = atmo%qv(i,k) - nuc_q

END IF
END IF
ENDDO
ENDDO

END SUBROUTINE ice_nucleation_homhet
Appendix B  Figures

Figure B.1: As Figure 13, but for experiment 3 (humidity threshold $S_{cr}$ reduction by 0.1).
Figure B.2: As Figure 13, but for experiment 1 (humidity threshold $S_{cr}$ reduction by 0.3).
Versicherung an Eides statt


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Ort, Datum             Christoph Sauter