

Standardized daily high-resolution large-eddy simulations of the Arctic boundary layer and clouds during the complete MOSAiC drift

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Abstract

This study utilizes the wealth of observational data collected during the recent MOSAiC drift experiment to constrain and evaluate 190 daily Large-Eddy Simulations (LES) of Arctic boundary layers and clouds at turbulence-resolving resolutions. A standardized approach is adopted to tightly integrate field measurements into the experimental configuration. Covering the full drift represents a step forward from single-case LES studies, and allows for a robust assessment of model performance against independent data under a broad range of atmospheric conditions. A homogeneously forced Eulerian domain is simulated, initialized with radiosonde and value-added cloud profiles. Prescribed boundary conditions include various measured surface characteristics. Time-constant composite forcing is applied, primarily consisting of subsidence rates sampled from reanalysis data. The simulations run for multiple hours, allowing turbulence and mixed-phase clouds to spin up while still facilitating direct comparison to MOSAiC data. Key aspects such as the vertical thermodynamic structure, cloud properties, and surface energy fluxes are satisfactorily reproduced and maintained. Specifically, the model captures the bimodal distribution of atmospheric states that is typical of Arctic climate. Selected days are investigated more closely to assess the model's skill in maintaining the observed boundary layer structure. The sensitivity to various aspects of the experimental configuration and model physics is tested. The model input and output are available to the scientific community, supplementing the MOSAiC data archive. The close agreement with observed meteorology justifies the use of LES data for gaining further insight into Arctic processes and their role in Arctic climate change.

1 **Standardized daily high-resolution large-eddy**
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8 **Key Points:**

- 9 • Campaign data is deeply integrated into the experimental design of daily turbulence-
10 and cloud-resolving simulations.
- 11 • Independent drift-long statistics on key aspects of the surface energy budget, ther-
12 modynamic structure, and clouds are reproduced.
- 13 • Sensitivities of the results to the experimental design and model physics are ex-
14 plored.

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Abstract

This study utilizes the wealth of observational data collected during the recent *MOSAiC* drift experiment to constrain and evaluate 190 daily Large-Eddy Simulations (LES) of Arctic boundary layers and clouds at turbulence-resolving resolutions. A standardized approach is adopted to tightly integrate field measurements into the experimental configuration. Covering the full drift represents a step forward from single-case LES studies, and allows for a robust assessment of model performance against independent data under a broad range of atmospheric conditions. A homogeneously forced Eulerian domain is simulated, initialized with radiosonde and value-added cloud profiles. Prescribed boundary conditions include various measured surface characteristics. Time-constant composite forcing is applied, primarily consisting of subsidence rates sampled from reanalysis data. The simulations run for multiple hours, allowing turbulence and mixed-phase clouds to spin up while still facilitating direct comparison to *MOSAiC* data. Key aspects such as the vertical thermodynamic structure, cloud properties, and surface energy fluxes are satisfactorily reproduced and maintained. Specifically, the model captures the bimodal distribution of atmospheric states that is typical of Arctic climate. Selected days are investigated more closely to assess the model's skill in maintaining the observed boundary layer structure. The sensitivity to various aspects of the experimental configuration and model physics is tested. The model input and output are available to the scientific community, supplementing the *MOSAiC* data archive. The close agreement with observed meteorology justifies the use of LES data for gaining further insight into Arctic processes and their role in Arctic climate change.

Plain Language Summary

The Arctic is one of the regions most affected by global climate change, warming up to four times as fast as the rest of the globe. It is also a particularly inaccessible region to conduct measurements. Fortunately, between 2019 and 2020 the *MOSAiC* campaign collected an unprecedented amount of data in the Arctic. In this study, numerous of these measurements are incorporated into high-resolution computer simulations of the lowest part of the Arctic atmosphere. This simulation data complements and contextualizes the observations and enables insight into complex physical processes, e.g., cloud formation, ice production, or turbulent mixing. The Arctic is an extreme place, and models often struggle to represent the atmosphere accurately. Therefore, the main achievement of this study is to successfully simulate 190 atmospheric situations as measured during the campaign. The generated data set performs well when compared to independent observations. Single cases deliver information about individual atmospheric conditions, and the collection gives insight into how key climate variables behaved throughout the *MOSAiC* year.

1 Introduction

The ongoing rapid warming of the Arctic region is a significant contributor to global climate change. Due to amplification processes, the Arctic warms up to four times as fast as the rest of the globe (Serreze & Barry, 2011; Rantanen et al., 2022). Past research suggests various feedback processes cause this Arctic Amplification (AA) (Wendisch et al., 2023), including the albedo (Screen & Simmonds, 2010; Thackeray & Hall, 2019; Dai et al., 2019; Jenkins & Dai, 2021), Planck (Pithan & Mauritsen, 2014), water-vapor, lapse rate (Stuecker et al., 2018; Linke et al., 2023), and cloud feedback (Philipp et al., 2020; Middlemas et al., 2020). To better understand these feedback mechanisms, it is crucial to quantify the effects of turbulent boundary layer processes in the Arctic atmosphere amid a changing climate (Taylor et al., 2018). Furthermore, it is essential to inform large-scale model parameterizations with high-resolution modeling efforts. Here, a collection of 190 of these numerical experiments is created by integrating a variety of Arctic measurements.

The investigation of the high Arctic is highly challenging for various reasons. The dynamic sea-ice masses make it impossible to install permanent measuring stations. Therefore, reliable meteorological data from ship- and airborne measurement campaigns and satellite imagery is sparsely available. All of which suffer from spatial and temporal gaps in the coverage. The *Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC, Shupe et al. (2020))* was a major international field campaign that took place in the Arctic from September 2019 to October 2020, intending to fill essential data gaps in in-situ observations in the central Arctic, covering an entire annual cycle. The campaign involved the deployment of the German research vessel *Polarstern*, which was frozen into the Arctic sea ice and drifted with it for over a year. During this time, the campaign and connected projects gathered an unprecedented amount of highly diverse data sets and made them available to the research communities in atmospheric, cryospheric, and oceanic sciences (Shupe et al., 2022; Nicolaus et al., 2022; Rabe et al., 2022).

The first objective of this work is to integrate available observational data sets from the *MOSAiC* campaign into a high-resolution numerical experiment. This supplements the data record with time-resolved three-dimensional modeling results and augments singular data sets by contextualizing their role in a turbulent boundary layer. A quantity of high-resolution Large Eddy Simulations (LES) are performed to achieve this.

LES is valuable for resolving critical small-scale boundary layer processes, including cloud dynamics and turbulence. This method also employs well-established parameterization techniques for surface energy exchange and micro-physical processes to facilitate the simulation of larger domains, allowing for the formation of mesoscale structures. LES has been extensively utilized in boundary layer research for several decades - also in the Arctic region. Granted, past model intercomparison studies show weaknesses and strong sensitivities in representing (mixed-phase) cloud properties (Klein et al., 2009; Fridlind et al., 2012; Ovchinnikov et al., 2014; Stevens et al., 2018) and there is strong evidence suggesting a high spatial resolution is needed to accurately represent the turbulent dynamics in a rather energy-sparse Arctic atmosphere (van der Linden et al., 2020; van der Linden & Ansorge, 2022). Nonetheless, there have been several additional successful studies using LES for Arctic boundary layer research (e.g., Solomon et al. (2011); Morrison et al. (2011); Neggers, Chylik, et al. (2019); Egerer et al. (2021); Chylik et al. (2023)): This demonstrates the importance of a careful setup to achieve an accurate representation of the Arctic atmosphere in a virtual domain. The amount of *MOSAiC* datasets enables a setup with a minimum of uncertainties as well as a fair and thorough evaluation of the results.

The overarching goal of this particular work is to create a suit of 190 high-resolution LES representing the conditions of the lower Arctic atmosphere throughout the whole *MOSAiC* year. The choice of days was purely taken based on sufficient data availability. This approach has two main objectives: First, learn about the Arctic climate system, especially smaller-scale processes that are difficult to measure reliably and can hardly be accurately represented in larger-scale models. Second, identify weaknesses in the model

107 under different conditions by evaluating the simulation results against a large amount
 108 of diverse *MOSAiC* data sets. Therefore, keeping a standardized setup for each case is
 109 crucial to discovering systematic framework or parameterization problems. Initial and
 110 boundary conditions, model settings, and evaluation are all done without any manual
 111 adjustment on a case-to-case basis. The approach taken in this work sets it apart from
 112 individual case studies that prioritize optimizing single simulations at the expense of gain-
 113 ing a broader understanding of the model’s potential weaknesses, which a highly customized
 114 configuration may mask. It also enables the creation of impact studies for a diverse li-
 115 brary of cases by modifying this standardized setup.

116 The idea of standardized multi-month/multi-year LES has been successfully em-
 117 ployed at different super-sites where continuous data is available, e.g., at Cabauw, Nether-
 118 land (Neggers et al., 2012; Schalkwijk et al., 2015), at JOYCE, Germany (van Laar et
 119 al., 2019), within the LASSO project (Gustafson Jr et al., 2020) or even in more north-
 120 ern places as Svalbard (Kiszler et al., 2023). The *Polarstern* and the surrounding mea-
 121 surement stations act as a one-year super-site.

122 Section 2 gives a detailed description of the method, including an overview of the
 123 datasets used, the numerical model framework, and the configuration of the experiments
 124 based on the *MOSAiC* data. The results of the simulation and their evaluation against
 125 measurements are presented in section 3. A detailed discussion of the results’ meaning,
 126 implications, and limitations is found in section 4. Finally, section 5 summarizes the main
 127 conclusions of this study and provides an outlook on future research it might inspire.

128 2 Data and Method

129 2.1 *MOSAiC* datasets

130 At the foundation of the drift-covering library of high-resolution Large Eddy Sim-
 131 ulations of the Arctic atmospheric boundary layer discussed in this study are the obser-
 132 vational datasets collected during the *MOSAiC* drift. Table 1 gives a complete overview
 133 of these data. It includes the variable, its units and full name, the dimensionality, the
 134 associated instrument, and the scientific study presenting the dataset. We refer to these
 135 publications for a more detailed technical and scientific description of these datasets and
 136 the associated instruments.

137 Vertical profiles of the thermodynamic state, including temperature and water va-
 138 por specific humidity, are provided by the daily 11:00 UTC radiosonde launches during
 139 the *MOSAiC* campaign (Maturilli et al., 2022; Dahlke et al., 2023). Vertical cloud liq-
 140 uid and ice water content profiles are obtained from the value-added cloud product based
 141 on remote sensing datasets as described by Shupe et al. (2015). Information on cloud
 142 condensation nuclei concentrations is based on aerosol measurements (Koontz et al., 2020),
 143 while ice nucleating particle concentrations are based on the aerosol measurements by
 144 Creamean (2022). The skin temperature of the sea ice is based on the brightness tem-
 145 perature measurements from the *MetCity* location on the sea ice (Cox et al., 2023; Cox
 146 et al., 2023). Also based on tower measurements are estimates of the surface aerodynamic
 147 roughness length (Gallagher, 2023). Finally, surface albedo values are obtained from satel-
 148 lite products (Spreen et al., 2008; Istomina et al., 2020).

149 A few datasets required for the configuration of the daily numerical experiments
 150 are not mentioned in Table 1 because they are based on *ERA5* reanalysis data (Hersbach
 151 et al., 2018a, 2018b, 2023). These include vertical profiles of horizontal wind and time
 152 series of the sea-ice fraction. The motivation for using reanalysis products for these vari-
 153 ables is to make the simulated domain reflect a larger area and avoid introducing ultra-
 154 local effects. A few variables are also derived from *ERA5* because they were not mea-
 155 sured during the *MOSAiC* drift. These include large-scale vertical motion (subsidence)

156 and pressure gradients, adopting the procedure implemented by Neggers, Chylik, et al.
157 (2019); van Laar et al. (2019).

158 The resulting simulations are evaluated against additional *MOSAIC* datasets in-
159 dependent from those used in the experimental design. Simulated short- and longwave
160 radiative fluxes are compared to sensor data of the radiation station described by Cox
161 et al. (2023) and Riihimaki (2021). This installation was part of *MetCity* with sensors
162 placed at 3 m (upwelling) and 1.5 m (downwelling) height. Simulated near-surface tur-
163 bulent heat fluxes are evaluated against data described by Cox et al. (2023), who dis-
164 cuss two different heat flux datasets. One is directly retrieved from sonic-anemometer
165 turbulence measurements, while the other is a bulk calculation based on Monin-Obukhov
166 theory. The latter is used in this study, although Cox et al. (2023) do mention poten-
167 tial over-simplifications, such as the assumption of constant roughness lengths. Since the
168 surface flux parameterization in the model is also based on Monin-Obukhov theory, the
169 use of bulk measurements yields the fairest comparison of the model to data.

170 2.2 Model setup

171 2.2.1 *LES* code

172 The *Dutch Large Eddy Simulation* framework (*DALES*, Heus et al. (2010)) was uti-
173 lized in this research. This code has been effectively employed in numerous boundary
174 layer studies (de Roode et al., 2016; Van der Dussen et al., 2013; van Laar et al., 2019),
175 particularly also to conduct Arctic research (Neggers, Chylik, et al., 2019; de Roode et
176 al., 2019; Chylik et al., 2023; Egerer et al., 2021). The foundation of the model is the
177 Ogura-Phillips anelastic equations for a set of prognostic variables, including liquid wa-
178 ter potential temperature Θ_1 , the velocity components $\{u, v, w\}$, total water specific hu-
179 midity q_t , and the mass concentration as well as number concentration of various hydrom-
180 eteor species. Momentum advection is calculated by a fifth-order central difference scheme
181 and scalar advection by a κ -limiter scheme (Hundsdoerfer et al., 1995). A prognostic TKE
182 model calculates the subgrid-scale transport of heat, moisture, and momentum. Finally,
183 the time integration makes use of a 3rd-order Runge-Kutta scheme. To better represent
184 mixed-phase clouds in a wide range of conditions, we enhanced the cloud microphysics
185 scheme, the radiation scheme, and the surface scheme, as described in more detail be-
186 low.

187 2.2.2 *Microphysics*

188 The mixed-phase, double-moment micro-physics scheme by Seifert and Beheng (2006)
189 has enabled the inclusion of ice-cloud processes in investigations of the Arctic climate
190 system and has been used in various research projects and models (Schemann & Ebell,
191 2020; Kiszler et al., 2023; Chylik et al., 2023; Linke et al., 2023). It considers the mass
192 and number concentration of five hydro-meteors: Cloud droplets and cloud ice crystals
193 and the precipitating hydro-meteors snow, graupel, and rain. The cloud condensation
194 nuclei concentration is single-species and prognostic, while the ice nucleating particle con-
195 centration is also single-species but prescribed, and its activation depends on temper-
196 ature. The microphysics scheme was initially designed for simulating ice clouds in the
197 mid-latitudes and, therefore, requires evaluation and partial adaptation to suit the ex-
198 tremely cold conditions in the high Arctic. Two key changes to the original implemen-
199 tation (Chylik et al., 2023) were made: Firstly, we calculate the heterogeneous freezing
200 rates using the maximum of the actual atmospheric temperature and $T_{\text{het,lim}} = -15^\circ\text{C}$,
201 as temperatures below this threshold lead to the edges of the valid range of the param-
202 eterization being approached and exceeded (Pruppacher & Klett, 1996). Secondly, the
203 maximum number concentration of nucleated ice particles produced by deposition-nucleation
204 is limited to $c_{N,\text{ice}} = 200 \text{ L}^{-1}$ to prevent an unrealistically high concentration of tiny
205 ice particles, which would exceed the estimated concentration of available ice nucleat-

Table 1. Overview of observational data sets utilized to set, constrain, and evaluate the conducted simulations.

Variable	Unit	Description	Dimension	Instrument	Citation
α	%	Surface albedo	(t)	AMSR-E Satellite	Spreen et al. (2008); Istomina et al. (2020)
q_v	kg kg^{-1}	Water vapor specific humidity	(z, t)	Radiosonde	Maturilli et al. (2022); Dahlke et al. (2023)
Θ_v	K	Virtual potential temperature	(z, t)	Radiosonde	Maturilli et al. (2022); Dahlke et al. (2023)
q_l	kg kg^{-1}	Liquid water specific humidity	(z, t)	Multi-sensor retrieval	Shupe et al. (2015)
q_i	kg kg^{-1}	Ice water specific humidity	(z, t)	Multi-sensor retrieval	Shupe et al. (2015)
LW_d	W m^{-2}	Longwave downward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
LW_u	W m^{-2}	Longwave upward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
SW_d	W m^{-2}	Shortwave downward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
SW_u	W m^{-2}	Shortwave upward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
T_{skin}	K	Skin temperature	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
$U_{10\text{m}}$	m s^{-1}	10 m wind speed	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$T_{10\text{m}}$	K	10 m temperature	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$H_{s,10\text{m},\text{bulk}}$	W m^{-2}	10 m Bulk sensible heat flux	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$H_{s,10\text{m},\text{turb}}$	W m^{-2}	10 m Turbulent sensible heat flux	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$z_{0,m}$	m	Roughness length for momentum	(t)	Meteorological tower	Cox et al. (2023); Gallagher (2023)
c_{CCN}	m^{-3}	Cloud condensation nuclei concentration	(t)	ARM optical particle counter	Koontz et al. (2020)
c_{INP}	m^{-3}	Ice nucleating particle concentration	(t)	DRUM aerosol sampler	Creamean (2022)

206 ing particles. However, these limits do not apply to the secondary production of ice. It
 207 is worth noting that developing an accurate microphysics scheme for the Arctic is a highly
 208 researched topic (Fridlind et al., 2012; Ong et al., 2022) that cannot be covered within
 209 the scope of this study, but by including the mentioned changes, realistic ice production
 210 has been achieved.

211 **2.2.3 Radiation**

212 By default, *DALES* uses a four-stream solver based on (Fu & Liou, 1993; Liou et
 213 al., 1988) in combination with Monte Carlo Spectral Integration (Pincus & Stevens, 2009)
 214 to calculate the vertical component of the radiative fluxes in the short- and longwave.
 215 Previously, the optical properties of ice water content in the radiation calculation were
 216 estimated to be identical to a liquid water content of the same mass and a prescribed
 217 constant number concentration. While this was expected to introduce an inevitable er-
 218 ror in general, it proved to be an unusable assumption for thin ice clouds in the Arctic.
 219 For this work, the description of the optical properties of ice crystals followed Fu and
 220 Liou (1993). This parameterization was developed for cirrus ice clouds with effective ice
 221 diameter in the range 20 – 120 μm .

222 Prior to this study the *DALES* code had never been applied to central Arctic con-
 223 ditions. A necessary step was to supply the radiation scheme with realistic information
 224 about the effective diameter of ice crystals. These are here based on the physical prop-
 225 erties of ice crystals (McFarquhar & Heymsfield, 1998; Baran, 2005), as estimated from
 226 the microphysics scheme. How microphysical properties of ice crystals such as size, ge-
 227 ometry, and density can be linked to radiative properties is not yet fully understood, and
 228 is an active research topic (Ryan, 2000; Mitchell, 2002; Konoshonkin et al., 2017; Ham
 229 et al., 2017). For this reason, the mean particle diameter calculated by the microphysics
 230 bulk scheme is for simplicity directly used as the radiative effective diameter. This sim-
 231 plification should be kept in mind when interpreting the results presented in this study.
 232 Testing more complex models for the effective diameter of ice particles in the LES is for
 233 now considered a future research topic.

234 Finally, two further simplifications in the treatment of radiation should be men-
 235 tioned. Firstly, in grid boxes with a mean ice crystal size outside of the range defined
 236 above, the effective diameter is set to the upper (respectively lower) bound. Secondly,
 237 the solar zenith angle is set constant for the duration of each simulation, and is calcu-
 238 lated based on the location and time of the radiosonde used for initialization of the model.
 239 The zenith angle affects the solar radiation, but three-dimensional effects are not con-
 240 sidered, and radiative transfer works purely in the vertical.

241 **2.2.4 Surface parameterization**

The parameterization of surface processes, particularly flux calculations, becomes
 necessary when using *DALES* due to the unresolved surface-roughness scale. Assuming
 that the first model level lies in the atmospheric surface layer, computing the exchange
 between atmosphere and surface becomes possible based on the Monin-Obukhov theory
 and the surface layer bulk Richardson number Ri_B (Louis, 1979):

$$242 Ri_B = \frac{z_1}{L} \frac{\left[\ln \frac{z_1}{z_{0,h}} - \Psi_H \left(\frac{z_1}{L} \right) + \Psi_H \left(\frac{z_{0,h}}{L} \right) \right]}{\left[\ln \frac{z_1}{z_{0,m}} - \Psi_M \left(\frac{z_1}{L} \right) + \Psi_M \left(\frac{z_{0,m}}{L} \right) \right]^2}. \quad (1)$$

243 Here, z_1 is the height of the first model level, L the Obukhov length, $z_{0,h}$ and $z_{0,m}$ the
 244 roughness lengths for heat and momentum, respectively, and Ψ_H and Ψ_M the integrated
 245 stability functions. For a more detailed description refer to Heus et al. (2010).

246 The stability functions for the unstable and neutral conditions are unchanged from
 the initially released code base, while for the stable conditions, the stability functions

247 by Grachev et al. (2007) are newly implemented. They were specifically developed for
 248 the Arctic regime based on data from the SHEBA campaign suiting this application. The
 249 use of roughness lengths derived from MOSAiC measurements is discussed in section 2.3.4.

250 Originally, the computation of sensible and latent heat fluxes at the surface relied
 251 on a single uniform surface skin temperature. However, a slightly different approach was
 252 introduced, which considers two distinct skin temperatures: the ice skin temperature mea-
 253 sured and the ocean skin temperature set to $t_{\text{skin,ocean}} = -1.8^\circ\text{C}$. By computing fluxes
 254 for both temperatures and then taking a weighted average based on the sea-ice fraction,
 255 this approach allows for partial inclusion of open ice effects into the simulation. If the
 256 ice temperature exceeded -1.8°C , ocean and sea-ice temperature were assumed to be
 257 identical.

258 The ice skin temperature is prescribed and constant throughout the simulation. This
 259 one-way surface-atmosphere coupling reduces the complexity of the simulation immensely,
 260 and the error it introduces is expected to be minimal, primarily because of relatively short
 261 simulation times.

262 **2.3 Experimental configuration**

263 *2.3.1 Domain and grid*

The choice of domain and grid size is crucial for the quality of a simulation. The
 adopted spatial discretization reflects the limits computational resources impose on sim-
 ulating a full year at turbulence-resolving resolutions. Ensuring that turbulent structures
 are accurately represented is imperative, which requires a sufficient grid resolution. To
 avoid the unwanted effects of periodic boundaries in the horizontal directions, the do-
 main must be appropriately sized to provide mesoscale structures with enough space to
 evolve. In the standardized setup, the horizontal domain and grid utilized are:

$$L_x = L_y = 6400 \text{ m}$$

$$\Delta x = \Delta y = 20 \text{ m}$$

264 An Eulerian framework is adopted, with the domain fixed in space at the *Polarstern* lo-
 265 cation. This choice is motivated by our double objective of i) performing short-range sim-
 266 ulations lasting only a few hours and ii) being able to compare model results to station-
 267 ary measurements.

268 The top of the vertical domain is at $L_z \approx 12 \text{ km}$. The lowest 1200 m of the field
 269 is resolved with a grid spacing of $\Delta z_{\text{min}} = 10 \text{ m}$. Above this level, the grid spacing in-
 270 creases exponentially with height until a maximum grid spacing of $\Delta z_{\text{max}} = 185 \text{ m}$. The
 271 non-regular vertical grid allows for high resolution in the cloud-containing boundary layer
 272 while also accommodating tropospheric features such as higher-level clouds that primar-
 273 ily exert radiative effects on the lower domain. In total, the grid consists of 286 verti-
 274 cal levels. For a more detailed description refer to Appendix A

275 In the process of finding a compromise between domain size and resolution with
 276 fixed available computational resources, it was decided to prioritize resolution: The $6.4 \text{ km} \times$
 277 6.4 km domain is enough to allow for thermodynamic heterogeneities in the virtual area
 278 but might lack the evolution of larger mesoscale structures. Since this work is focused
 279 on accurately representing realistic conditions and smaller-scale processes in the Arctic
 280 atmospheric boundary layer, the resolution that has been selected is satisfactory. The
 281 small grid boxes, especially in the lowest layers, enable an accurate representation of tur-
 282 bulance and all turbulence-driven processes, e.g., cloud evolution and life cycle, entrain-
 283 ment, shear-layer mixing, detailed distribution of microphysical interactions, surface fluxes,
 284 etc. This setup is referred to as PRODUCTION setup in the following.

285 A second configuration (TEST) was employed: By reducing the horizontal domain
 286 to $800 \text{ m} \times 800 \text{ m}$ and the horizontal resolution to $25 \text{ m} \times 25 \text{ m}$ the computational ex-
 287 pense is reduced drastically. The vertical grid is kept unchanged. While this resolution
 288 and domain size decrease the simulation quality, the results are still greatly informative.
 289 The TEST configuration proved to be crucial in curating and testing the standardized

290 setup and the integration of measurements in an efficient manner. This procedure of us-
 291 ing micro-grids to inform the setup of expensive runs was inspired by Neggers, Chylik,
 292 et al. (2019). Table 2 summarizes the two setups.

Table 2. Resolution and domain size for different setups.

Setup	Resolution (h × v)	Domain (h × v)	Usage
PRODUCTION	20 m × (10 – 185 m)	6.4 km × 12 km	Definitive runs
TEST	25 m × (10 – 185 m)	0.8 km × 12 km	Impact studies

293 **2.3.2 Initial profiles**

294 The initial conditions of each simulation are mostly derived from data gathered dur-
 295 ing the *MOSAiC* campaign to constrain the experiments as much as possible with mea-
 296 surements. All initial profiles, most of which concern prognostic variables in the model,
 297 are horizontally homogeneous in the simulation domain.

298 Initial profiles of the two prognostic thermodynamical state variables in *DALES*,
 299 total water specific humidity q_t and liquid water potential temperature θ_l , are derived
 300 from data from the 11:00 UTC radiosonde launched at the *Polarstern* (Maturilli et al.,
 301 2022). Corrections were applied to account for elevated launch height and initial sen-
 302 sor adjustment after launch by Dahlke et al. (2023). For this purpose, the radiosonde
 303 data was combined with measurements from the *MetCity* meteorological tower (Cox et
 304 al., 2023). The prognostic model variables q_t and θ_l in the *DALES* code are derived from
 305 the radiosonde temperature, humidity, and pressure measurements. Further, for ice lay-
 306 ers, the derived q_v profile was bounded by the saturation specific humidity $q_{\text{sat},i}$, to limit
 307 the impact of measurement uncertainties on the sensitive initialization of ice clouds. The
 308 full procedure is detailed in Appendix B.

309 The two prognostic variables of suspended cloud mass, cloud liquid water content
 310 (LWC) and ice water content (IWC), are also initialized with measurement-based pro-
 311 files. In the *DALES* code, these variables are denoted as q_l and q_i , respectively. Initial-
 312 izing cloud variables with observations reflects our objective of simulating and resolv-
 313 ing small-scale turbulent variability around the *MOSAiC* instrumentation, which is of-
 314 ten driven by cloud processes. One could initialize with a cloud-free state and let mixed-
 315 phase clouds develop by themselves over time. However, previous LES intercomparison
 316 studies on mixed-phase clouds have shown that this is difficult to achieve in a short sim-
 317 ulation time (Neggers, Chylik, et al., 2019; Stevens et al., 2018), and the simulations tend
 318 to drift significantly away from the initialized atmospheric thermodynamic state as the
 319 clouds form. These points motivated the adoption of direct initialization of cloud mass.
 320 To achieve this, accurate placement and phasing of the initial cloud mass relative to the
 321 vertical atmospheric thermodynamic profile is imperative. Because cloud mass is not di-
 322 rectly measured by the radiosonde, the data product of Shupe et al. (2015) is used in this
 323 study. The multi-sensor cloud retrieval product features vertically resolved LWC and IWC
 324 at 1 min resolution. To ensure that extreme values are avoided and the overall thermo-
 325 dynamic state of the boundary layer is captured, the initial conditions used are mean
 326 LWC and IWC profiles. This approach focuses on representing the average conditions
 327 across the entire domain rather than the potential heterogeneities in certain areas. In
 328 each case, the 1 min profiles from the data set are averaged for 15 min after the radiosonde
 329 launch time, around 11:00 UTC, depending on the day. This time window is sufficient
 330 to average across individual cloud-turbulence elements yet brief enough to prevent al-
 331 terations in the overall large-scale atmospheric conditions.

332 The prognostic humidity budget equation in *DALES* is formulated in terms of $q_t =$
 333 $q_v + q_l$ as the total humidity and excludes suspended cloud ice which is treated as a sep-
 334 arate prognostic variable. To achieve an internally consistent initialization of all humid-

335 ity state variables, q_v , q_l , and q_i are combined in a height-dependent way, as follows. In
 336 areas of expected turbulent ice production (below z_{cut} , see equation (B7)), the ice and
 337 liquid water specific mixing ratio are added and given to the model as only liquid. The
 338 expected behavior of the model is to convert the additional liquid into ice via the mi-
 339 crophysics scheme and represent accurate IWC and LWC distributions after a spin-up
 340 phase. In areas of expected deposition ice production (above z_{cut}), the retrieved IWC
 341 is directly included in the model. If ice is measured, the model will place ice clouds di-
 342 rectly with an estimated effective radius of $55 \mu\text{m}$. This shortens the lengthy deposition
 343 spin-up process and produces realistic, weakly turbulent, high-level ice clouds.

344 The initial profile of the cloud condensation nuclei (CCN) concentration in the *DALES*
 345 mixed-phase microphysics scheme (see 2.2.2) are estimated based on the observations
 346 from the *Cloud Condensation Nuclei Particle Counter* located aboard *Polarstern* (Koontz
 347 et al., 2020). The measurements show high seasonal and day-to-day variability, as well
 348 as variability during some days. However, with an emphasis on the consistency of the
 349 setup, the mean value of each day is used as the initial value of CCN concentration for
 350 the simulation. The value from the preceding recorded day was used for days missing
 351 data. In the absence of a consistent CCN profiling of the Arctic air, the measurements
 352 in the bottom part of the atmosphere are considered a good proxy for the conditions in
 353 the rest of the boundary layer.

354 The number concentration of activated ice nucleating particles (INP) is not yet treated
 355 prognostically in the current version of the *DALES* microphysics scheme. In the code,
 356 the INP concentrations are determined from temperature-dependent activation spectra
 357 (Seifert & Beheng, 2006), prescribed by exponential functions with constant parameters
 358 proposed by Reisner et al. (1998). Laboratory measurements of INP activation from in-
 359 situ samples of Arctic air extracted near *Polarstern* during *MOSAIC* (Creamean et al.,
 360 2018; Creamean, 2022) showed a high time-variation in activation spectra, motivating
 361 initialization with daily observed values. The associated observed INP number concen-
 362 trations were significantly lower than the values proposed by the parameterization men-
 363 tioned above, often by more than two orders of magnitude. To keep the simulations as
 364 representative as possible of the observed atmosphere, the measured activation spectra
 365 were used instead. A logarithmic regression was applied to each measured spectra from
 366 the laboratory samples, and the resulting slope and intercept parameters were then in-
 367 serted as new values in the deposition-nucleation scheme instead of the original constant
 368 values. Finally, limitations in the sampling of the spectra during the drift necessitate adopt-
 369 ing two further simplifications in the initialization of the INP profile in the model. Firstly,
 370 due to the three-day sampling rate, the spectra on sampling-free days are set at the val-
 371 ues from the last preceding day of availability. Secondly, due to the absence of consis-
 372 tent and continuous INP profiling during the drift, the activation spectra are simply as-
 373 sumed constant with height.

374 **2.3.3 Lower boundary conditions**

375 Similar to the initial profiles, the lower boundary conditions for model variables
 376 are mainly based on *MOSAIC* data. Additional information is taken from the ERA5 re-
 377 analysis. The boundary conditions are prescribed, constant in time, and horizontally ho-
 378 mogeneous in the simulated domain.

379 The sea-ice fraction at the location of the *Polarstern* is taken from ERA5 reanal-
 380 ysis data. With the research vessel frozen in solid pack ice for most of the simulated days,
 381 the sea-ice fraction at the ship was often close to 100 %. Accordingly, short-time reduc-
 382 tions in the sea-ice fraction, for example, due to lead events, are not considered in the
 383 control experiments for simplicity but could simply be added in future sensitivity exper-
 384 iments.

As described in section 2.2.4, two surface skin temperatures are considered in the
DALES bulk surface parameterization; one for sea ice and one for open water. For the
 ice surface skin temperature T_{seaice} the brightness temperature measurements at the *MetC-*

ity installation are used (Cox et al., 2023). For the skin temperature of open water, the ocean temperature is used, which is assumed to follow

$$T_{\text{ocean}} = \max(T_{\text{seaice}}, -1.8^\circ\text{C}), \quad (2)$$

385 where the numeric value represents the typical freezing temperature of ocean water. In
 386 practice, and for consistency with the profile initialization described above, for T_{seaice}
 387 the surface value of the combined data product by Dahlke et al. (2023) is used. This value
 388 is the skin temperature measured at *MetCity*. Preliminary experiments demonstrated
 389 that the skin temperature is a crucial boundary condition to get right, as it directly de-
 390 termines the upward longwave radiation and strongly affects the low-level stability in the
 391 simulations. For this reason, no simulations were carried out for days on which *MetC-*
 392 *ity* data were not available. Using *ERA5* values as a replacement was no option for these
 393 days because i) this would introduce inconsistencies in the boundary conditions during
 394 the drift, and ii) warm biases are known to exist in the reanalysis regarding the surface
 395 skin temperature (Day et al., 2020). As a guiding principle, integrating different data
 396 sets in the simulation for the same quantity goes against the approach of a standardized
 397 setup.

398 **2.3.4 Surface properties**

399 The surface roughness length for momentum $z_{0,m}$ plays a key role in the Monin-
 400 Obukhov theory for calculating turbulent fluxes. Accordingly, adopting realistic values
 401 is important to get the flux boundary condition right. However, in many model appli-
 402 cations, including LES research, the surface roughness length is simply estimated, e.g.,
 403 ECMWF (2021); Michaelis et al. (2020). Fortunately, $z_{0,m}$ can be derived from daily *MO-*
 404 *SAiC* data of the near-surface wind, turbulence, and temperature measurements (Cox
 405 et al., 2023; Gallagher, 2023). This data provides an accurate boundary condition for
 406 $z_{0,m}$ for each simulated day. In the literature the surface roughness length for heat $z_{0,h}$
 407 in the Arctic is often assumed as $z_{0,h} = 0.1 \cdot z_{0,m}$ (e.g. IFS Model ECMWF (2021);
 408 Michaelis et al. (2020)). For lack of direct measurements of $z_{0,h}$ during the drift, this value
 409 is also adopted here for the control experiments.

410 The final boundary condition to be considered concerns the surface albedo α . Dur-
 411 ing polar day, the reflectivity of the predominantly frozen surface directly controls the
 412 solar contribution to the surface energy budget. The horizontal scale that α represents
 413 is set by the horizontal dimension of the simulated domain. Landscape features such as
 414 melt ponds and leads are known to affect the average reflectivity of an area on a meter
 415 to kilometer scale (Niehaus et al., 2023), while Arctic weather also influences surface prop-
 416 erties on much larger scales. To capture both effects at once, the satellite α product de-
 417 scribed by Spreen et al. (2008); Istomina et al. (2020) is adopted here. Two main issues
 418 affect the accuracy of the satellite estimates of surface albedo; cloud cover and limited
 419 satellite overpasses. As a result, satellite albedo products often have significant spatial
 420 and temporal gaps. To address this, a rolling average over a week-long period is used to
 421 smooth out as many inconsistencies as possible in the data. Secondly, spatial interpola-
 422 tion in the resulting maps gives a reasonable estimate of the albedo in areas around
 423 *Polarstern*. It is possible, that the interpolation in time and space introduces an albedo
 424 bias toward cloud-free conditions. A further improvement was not considered for two rea-
 425 sons. Albedo measurements for cloudy conditions would be derived from a second dataset,
 426 which clashes with the standardized setup. Secondly, the uncertainty by this bias is ex-
 427 pected to be small when used in the simplified radiation scheme employed in *DALES*.

428 **2.3.5 Large-scale forcing and nudging**

429 The simulated portion of the atmosphere is not isolated from the larger-scale flow
 430 in which it is embedded. Various larger-scale processes impact the development of the
 431 atmospheric boundary layer, including large-scale advection, vertical motion, and pres-
 432 sure gradients. In *DALES*, these forcings are considered and applied in a horizontally

433 uniform way, while maintaining height-dependency. The associated tendencies are either
 434 fully prescribed or partially interactive with the domain-average profile. This forcing method
 435 is described in detail by van Laar et al. (2019) and is, in principle, adopted here, with
 436 a few notable exceptions as described below.

In the prognostic budget equations for $\varphi \in \{q_t, \theta_1, u, v\}$ the tendency due to large-scale subsidence S_φ^{subs} is constructed using a prescribed large scale vertical motion w_s and the local vertical gradient, calculated from the vertical profile of the domain averaged variable $\bar{\varphi}$,

$$S_\varphi^{\text{subs}} = -w_s \frac{\partial \bar{\varphi}}{\partial z} \quad (3)$$

(Siebesma et al., 2003). This means the significant impact of subsidence on inversions is captured. In the momentum equations the pressure gradient (p) and Coriolis (f) forces are represented in combination, through the departure of the actual wind from the geostrophic wind,

$$S_u^{\text{p+f}} = -f(\bar{v} - \bar{v}_g), \quad (4)$$

$$S_v^{\text{p+f}} = f(\bar{u} - \bar{u}_g), \quad (5)$$

437 with f the latitude-dependent Coriolis parameter and subscript g indicating the geostrophic
 438 state. The latter is calculated from the horizontal pressure fields from ERA5.

439 In the standardized case generation, the time and location of the *Polarstern* at 11:00
 440 UTC are determined first. Then the six-hour upstream trajectory of the 950 hPa air mass
 441 is estimated from the ERA5 reanalysis data. The quantities required for calculating the
 442 forcing terms are then calculated at all trajectory points across an area of 1×1 degrees,
 443 using the Lagrangian perspective described by Neggers, Chylik, et al. (2019). This means
 444 all horizontal advective terms are zero per definition at the height of diagnosis (950 hPa).
 445 Finally, the forcing terms are then time-averaged over six hours preceding the arrival of
 446 the low-level air mass at the *Polarstern*. This yields time-constant composite forcings,
 447 which express how the air mass was modulated by larger-scale processes during the pe-
 448 riod in which any clouds observed at the *Polarstern* formed. To limit the influence of large-
 449 scale processes on the evolution of the simulated domain, horizontal advection of tem-
 450 perature and moisture is set to zero. This approach isolates boundary layer processes
 451 as drivers of atmospheric changes.

Continuous Newtonian nudging is applied above the boundary layer thermal in-
 version to prevent excessive drift of the upper part of the troposphere (Randall & Cripe,
 1999; Sobel & Bretherton, 2000; Derbyshire et al., 2004; Neggers et al., 2012). The nudg-
 ing tendency S_φ^n is formulated in terms of the spatially averaged profiles (Heus et al., 2010;
 Neggers et al., 2012),

$$S_\varphi^n = -\frac{1}{t^n} (\bar{\varphi} - \varphi^n). \quad (6)$$

Here, $\bar{\varphi}$ is the horizontal mean of an arbitrary scalar, t^n is the nudging time scale, and φ^n is the profile towards which the model profile is relaxed, which in this case is the initial profile based on the corrected 11:00 UTC radiosonde data. The nudging time scale is set to $t^n = 10\,800$ s. It is only applied above the boundary layer height z_i , which is adaptively calculated based on the maximum liquid water potential temperature gradient. This method is well established in the literature, e.g., (Sandu & Stevens, 2011; Zhang et al., 2013; Neggers et al., 2017). Height z_i as used to define the bottom of the nudging layer is defined to be situated in a specified range, as follows:

$$z_i, \text{ where } \left. \frac{\partial \Theta_v}{\partial z} \right|_{z=z_i} = \max \left(\left. \frac{\partial \Theta_v}{\partial z} \right|_z \right), z \in [100 \text{ m}, 5000 \text{ m}] \quad (7)$$

452 This specification is a practical protection against artificially high gradients near the sur-
 453 face and the tropopause inversion.

454 The final external forcing to be discussed is the radiative forcing at the top of the
 455 simulated domain. The downward radiative fluxes at the model ceiling are calculated
 456 by including the part of the full radiosonde (initial) profile in the radiative flux calcu-
 457 lations that is situated above the ceiling. This way, impacts of the upper atmosphere on
 458 both longwave and shortwave radiative transfer are represented as a soft and interactive
 459 boundary condition.

460 3 Results

461 With the initialization, boundary conditions, and large-scale forcing thus defined,
 462 an experimental configuration is obtained with the following key characteristics;

- 463 • The simulated domain represents a statistical, homogeneously forced downscal-
 464 ing of the mean atmospheric column as observed daily at 11:00 UTC at the *Po-*
 465 *larstern* during *MOSAiC*;
- 466 • The recent history of the low-level air mass is represented through Lagrangian forc-
 467 ing;
- 468 • Time-composite forcing means the simulations can quasi-equilibrate, depending
 469 on the proximity to a balance in the prognostic budget equations;
- 470 • Resolved, small-scale boundary layer processes are free to evolve below the ther-
 471 mal inversion;
- 472 • Mixed phase clouds are allowed to spin up and interact with radiation, resolved
 473 dynamics, and prognostic aerosol.

474 This model configuration was arrived at after extensive testing on both smaller and larger
 475 grids. A three-dimensional volume rendering of a mixed-phase cloud that results from
 476 this setup is shown in figure 1 to illustrate that the turbulent dynamics in which these
 477 clouds are embedded are resolved to a high degree with this setup. The presentation of
 478 the results with this model setup is subdivided into three parts. Section 3.1 provides an
 479 overview of the successfully simulated cases during the year-long *MOSAiC* drift. Sec-
 480 tion 3.2 presents the statistical evaluation of the model output against a year of *MO-*
 481 *SAiC* data, and includes a brief initial discussion on data comparability. Section 3.3 fo-
 482 cuses in more detail on three selected days, to gain insight into the typical behavior of
 483 single simulations and to explore the potential use of the generated library of simulations
 484 for further scientific research.

485 3.1 Simulation overview

486 Figure 2 gives an overview of the days during the *MOSAiC* drift that were success-
 487 fully simulated in the PRODUCTION setup featuring the highest resolution and the largest
 488 domain, as described in Table 2. Here, success implies two things:

- 489 • The data needed for the standardized setup is complete and available at 11:00 UTC;
- 490 • No numerical issues occurred, and the simulation was completed successfully.

491 A subset of non-simulated days can be distinguished that is more or less randomly dis-
 492 tributed in time. On these days, typically, an observational dataset is missing that is part
 493 of the experimental setup. Two longer, continuous periods also exist that are not simu-
 494 lated; one in May-June 2020 and another in July-August. These coincide with the *Po-*
 495 *larstern* not being at the ice floe or *MetCity* not being operational. If not stated oth-
 496 erwise, all results discussed below represent the PRODUCTION setup.

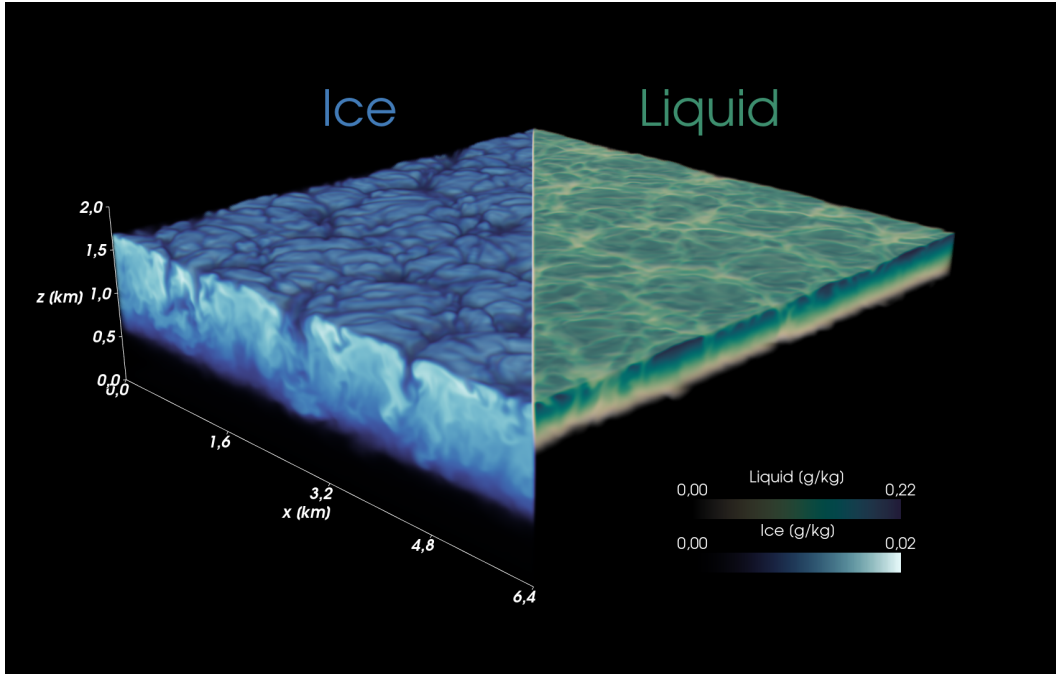


Figure 1. Volume rendering of the 20191101 case (see table 3) after 1.5 h of the full horizontal domain. The two quantities shown are the specific mixing ratios for ice (blue) and liquid (green) water. For visual reasons, the ice is only shown on the left, and the liquid only on the right.

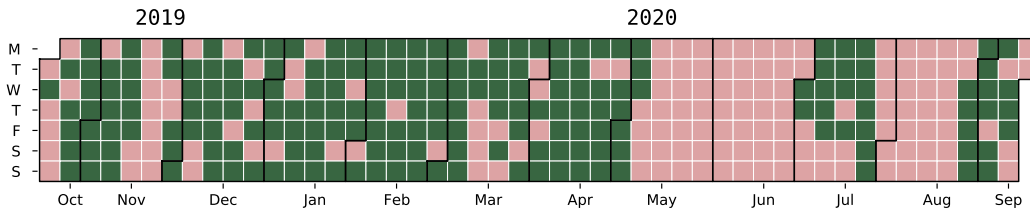


Figure 2. Overview of simulated case studies by date. Green indicates a successful simulation of the state of the boundary around 11:00 UTC at the *Polarstern*. Red shows days on which simulations were unsuccessful.

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3.2 Statistical evaluation

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The objective of this section is to evaluate the library of daily LES experiments against the year-long record of *MOSAIC* data. The general approach is to assess the difference between simulated values and their measured counterparts for selected variables to identify both strengths and weaknesses of the library of simulations concerning resolved aspects of the Arctic boundary layer and the surface energy budget. When interpreting the simulations and comparing them to measurements, three important considerations should be made, as briefly discussed here.

The first consideration is the *state of equilibrium* of the simulated and observed boundary layer. When the sum of all sources and sinks in the bulk ABL budget is non-zero, a net tendency exists that can gradually warm, cool, moisten, or dry the layer. Due to our lack of knowledge of these tendencies in nature, it remains unknown if the observed ABL is close to equilibrium or not. The simulated ABL can similarly be out of equilib-

rium, for example, through uncertainties in the applied forcings. However, what helps in model-observation comparability is the well-known slow adjustment of Arctic boundary layers, reflecting that net bulk tendencies are small compared to individual budget terms (Neggers, Chylik, et al., 2019). Another convenient factor is the observed persistence of ABL-related phenomena such as clouds (Shupe et al., 2006; Shupe, 2011; Stramler et al., 2011; Morrison et al., 2012), which implies that the model budget should be pretty similar to the observed one when initializing with observed cloud profiles. For these reasons, it is assumed a priori that the simulated ABL is, in principle, comparable to its observed equivalent. When doing so, one still needs to determine the optimal time point after initialization at which a comparison can be made. On the one hand, turbulent-cloudy processes need to spin up properly; on the other, significant drift from the desired state can happen and needs to be minimized. Careful equilibration analysis of all simulations yielded an optimal time point of 1.5 h after initialization. More details about this analysis can be found in Appendix C.

The second important consideration in the evaluation effort is the *independence of the observational data* from the numerical experiments. What is relevant is that the latter are already closely based on *MOSAIC* datasets. Ideally, one should evaluate resolved processes in the LES against completely independent datasets. This is indeed the case for a large subset of evaluation datasets, such as the surface radiative and turbulent energy fluxes. However, in principle, cloud properties are far less independent from the simulations, as these are initialized with observed cloud profiles. Nonetheless, it should be noted that clouds in the model can significantly evolve during the simulated period before the sampling time point due to strong interactions between thermodynamics, turbulence, and radiation. Accordingly, it is far from trivial that clouds remain unchanged from their initial state. This makes comparison to the observed cloud properties meaningful; a close agreement reflects model skill in maintaining the turbulent cloud layer.

The third consideration is about *uncertainties* in the observational datasets and how to deal with them in the model evaluation. A complicating factor is that these uncertainties also flow into the model setup through the initialization and boundary conditions. How these errors percolate into the final simulation, and to what degree, is hard to disentangle and even harder to isolate from other error sources such as numerics and the prescribed forcings. For these reasons, it was decided to exclude error bars in the evaluation plots. A thorough error analysis is for now considered future work.

3.2.1 Radiative energy fluxes

3.2.1.1 Longwave radiation Figure 3 shows scatter plots of the simulated versus observed near-surface longwave radiative fluxes at the *MetCity* site located on the ice floe near the *Polarstern* (Cox et al., 2023; Riihimaki, 2021). Included are the a) upward, b) downward, and c) net fluxes at 1–3 m height. The simulated upward flux reproduces the observed values to a high degree, in part because the surface skin temperature used in the simulations is derived from these radiation measurements. The good agreement confirms that the radiation scheme accurately represents the radiative energy emitted by the surface. A slight warm bias exists, which is introduced by the use of the double skin temperature as described in Section 2.3.3. The radiation scheme also uses this combined skin temperature (weighted by the sea-ice fraction) as the surface emission temperature for the wider area, while the measured fluxes purely reflect the local temperature of the (colder) sea ice on which they were made.

For the longwave downward flux (that indirectly reflects cloud presence) the agreement is also satisfactory, especially for the upper and lower tails of the distribution (Fig. 3b). This agreement indicates that the model does a reasonable job of simulating both the atmospheric temperature and the vertical location and presence of clouds. In the lower intermediate range, some positive outliers exist. To gain insight, Fig. 4 shows the same data but now shaded according to the (a) ice water path (IWP) and the (b) liquid water path (LWP). This additional information reveals that good agreement exists for i)

563 cold and cloud-free conditions ($LW_{\text{down}} \leq 120 \text{ W m}^{-2}$) as well as ii) warm and opti-
 564 cally thick liquid clouds ($LW_{\text{down}} \geq 200 \text{ W m}^{-2}$). The intermediate range suffers from
 565 a well-defined bias for relatively high IWP values, suggesting too high emissivity by thick
 566 ice clouds in the model. A deeper investigation of high-bias days revealed that the er-
 567 ror is introduced by parametric assumptions in the *DALES* radiation scheme concern-
 568 ing the effective diameter of ice crystals. An effective diameter range of 20–120 μm is
 569 applied, which was originally developed for cirrus clouds. Ice crystals in the Arctic can
 570 be observed to exceed that value (Shupe et al., 2006). Capping ice diameters at a too-
 571 small value leads to the overestimation of the optical thickness of ice clouds. Addition-
 572 ally, it is uncertain if the mean particle radius calculated by the bulk microphysics scheme
 573 can be used with proportional ratio 1 as the radiative effective radius in the radiation
 574 scheme. These sensitivities are discussed further in section 4.

575 Combining the upward and downward fluxes yields the net flux (Fig. 3c). The data
 576 shows the bimodal distribution typical of the Arctic, which is reproduced to a reason-
 577 able degree by the simulations and is explored in more detail in Section 3.2.4. While a
 578 general agreement exists with the observations, as expressed by the relatively low bias
 579 compared to the mean signal, the error introduced by the biases in the longwave down-
 580 ward radiation for ice clouds now materializes much more pronouncedly. Analysis indi-
 581 cates that the model particularly struggles in situations with optically thin ice clouds,
 582 claiming unrealistically low magnitude net radiative fluxes close to 0 W m^{-2} .

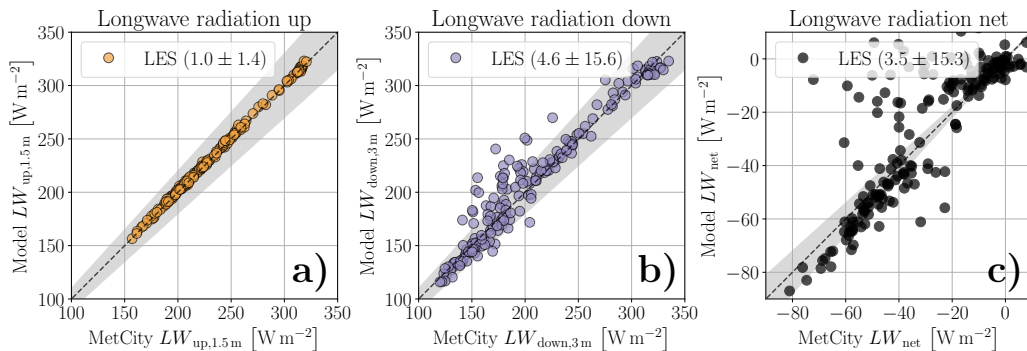


Figure 3. Scatter plots of simulated versus observed a) upward, b) downward, and c) net longwave radiative fluxes. LES results (ordinate) are plotted against *MetCity* tower measurements (abscissa). Each dot represents a single simulated daily case. The simulation is sampled at $t = 1.5 \text{ h}$ after initialization, while the measurement represents the 15 min average after radiosonde launch time. The dashed line indicates the one-to-one diagonal. The gray shading indicates the $\leq 10\%$ difference area, for reference. Values in the legend show $\mu \pm \sigma$, with μ and σ being the mean and standard deviation of simulated minus measured values, respectively.

583 **3.2.1.2 Shortwave radiation** Figure 5 compares the simulated and observed near-
 584 surface shortwave radiative fluxes. Non-zero values indicate polar spring and summer
 585 and reflect model performance during the melt season. When interpreting these results,
 586 it is important to realize that *DALES* only considers purely vertical radiative transfer.
 587 This assumption is commonly made in most atmospheric models, including most present-
 588 day LES codes, with only a few notable exemptions. However, it is also a significant sim-
 589 plification of reality that excludes three-dimensional radiative effects, which might in-
 590 troduce biases for low solar zenith angles, as are typical of the Arctic during polar day.
 591 With this in mind, the model biases in shortwave fluxes are largest at small values and
 592 decrease significantly as the shortwave fluxes increase. In terms of energy flux units, the

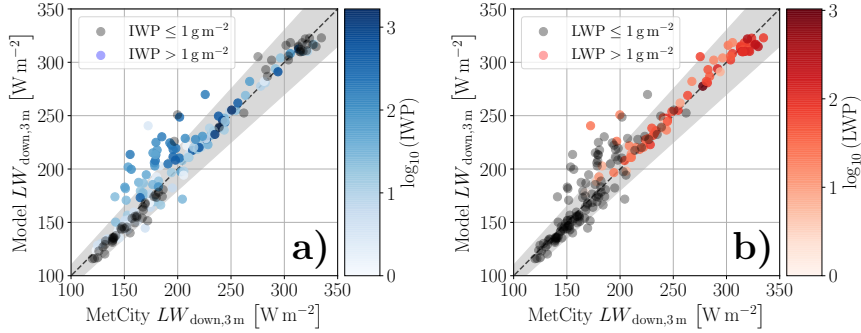


Figure 4. Similar to Fig. 3 b, but now shown with data points color-coded based on the simulated a) ice water path (IWP) and b) liquid water path (LWP).

593 bias and spread are somewhat larger compared to the longwave fluxes. For all three fluxes,
 594 the bias is negative, suggesting that too little shortwave energy is entering the system.
 595 This might be due to the exclusion of three-dimensional effects, a hypothesis that needs
 596 testing in future research. One notices that the distribution of data points in the upward
 597 and downward flux figures is structurally similar. In combination with the accuracy of
 598 the upward flux and in association with the resulting net flux, one concludes that the
 599 prescribed albedo boundary condition must be close to the true value. This skill was only
 600 arrived at after including the satellite-based albedo measurements (not shown).

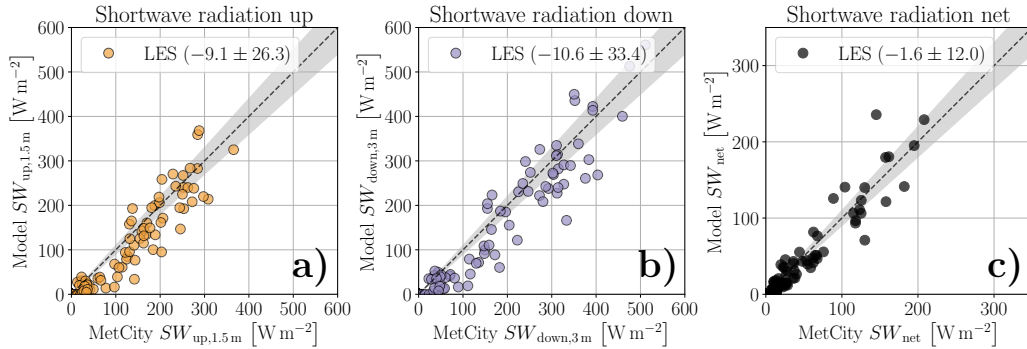


Figure 5. Similar to Fig. 3 but now showing the a) upward, b) downward, and c) net shortwave radiative flux at the surface.

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3.2.2 Water paths

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Two well-known and critical success metrics for reproducing clouds in the virtual domain are the liquid water path (LWP) and the ice water path (IWP). Figure 6 shows the comparison of simulated and measurement-based values for (a) IWP and (b) LWP. Focusing first on the ice, the general trend of measured IWP is well reproduced by the model. Measurements and model data agree for most cases. Nonetheless, several simulations under- or overestimate the amount of ice in the column. When interpreting these outliers it should be taken into account that the simulations are initialized with the observed profiles of liquid and ice cloud water. Accordingly, in these cases, the offsets arise during the simulated period, which points at the model experiencing difficulties main-

611 taining the right ice amount. Possible causes for this trend include i) lack of resolution
 612 to fully resolve cloud-forming dynamical processes in the upper atmosphere, ii) uncer-
 613 tainties in the applied large-scale forcings, and iii) lack of skill in the microphysics scheme.
 614 At this point, it is not clear which of these causes apply. However, encouraging aspects
 615 are that the model always maintains at least some ice and that the outliers seem ran-
 616 domly scattered around the correct mean as calculated over the full drift.

617 The measured LWP is mostly well captured by the simulations. A few cases un-
 618 derestimate the amount of liquid. This underestimate can happen when freezing rates
 619 are overestimated by the model and liquid clouds glaciate too eagerly. The most signif-
 620 icant relative errors for LWP and IWP occur in the region $\leq 50 \text{ g m}^{-2}$. Closer inspec-
 621 tion of these cases suggested that in situations with really thin ice and liquid clouds, the
 622 model is increasingly sensitive to the initial conditions. On the positive side, it can be
 623 considered a success that the model can capture and reproduce these thin clouds in the
 first place, to some degree.

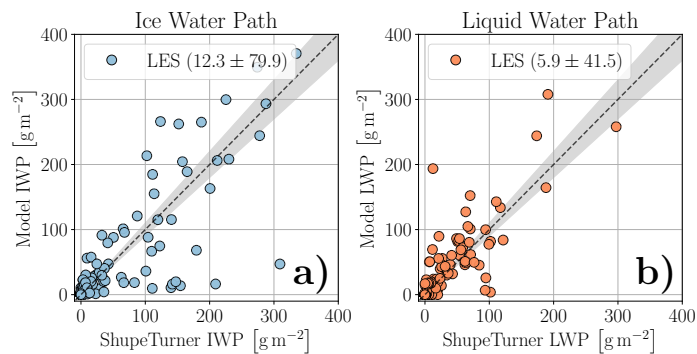


Figure 6. Scatter plot of simulated versus observed a) Liquid Water Path (LWP) and b) Ice Water Path (IWP). The LES is plotted against the ShupeTurner data set. Sampling, notation, and plotting style are analogous to the previous figures.

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625 3.2.3 Near-surface meteorology

626 Figure 7 shows the simulated versus observed (a) wind speed, (b) temperature, and
 627 (c) sensible heat flux at 10 m height. The wind speed in the simulation compares well
 628 to the measurements, which is especially gratifying since the wind profile given to each
 629 simulation as initial condition stems from *ERA5* reanalysis data. The *MOSAiC* radiosonde
 630 data were assimilated into *ERA5*. Simulation forcings and near-surface turbulence can
 631 cause differences from the initial profile after the spin-up phase. For these reasons, a good
 632 agreement is not trivial. Nonetheless, the relative error can be high for low wind speeds,
 633 and the impact on near-surface transport processes is significant. The simulation is bi-
 634 ased towards lower values for wind speeds $\geq 10 \text{ m s}^{-1}$. Low-level jets are a common phe-
 635 nomenon in the high Arctic (López-García et al., 2022), and their underestimation in
 636 the LES might explain this small bias.

637 Figure 7 b shows that the simulated 10 m temperatures closely resemble the ob-
 638 servations. This is arguably not surprising, given i) the prescribed observed skin tem-
 639 perature as measured at *MetCity* and ii) the radiosonde temperature profile being part
 640 of the model initialization. The close agreement at least confirms that the simulation has
 641 not drifted away from the measured thermodynamic state after the spin-up period.

642 Figure 7 c evaluates the simulated 10 m sensible heat flux (H_s). By convention, a
 643 positive sign indicates an upward flux. In general, the observed distribution and orien-

644 tation of the data points in this space are reproduced, but the mean bias and spread are
 645 relatively large compared to the mean signal. The mean bias is negative, expressing a
 646 general underestimation of the flux of sensible heat between surface and atmosphere. Sig-
 647 nificant negative biases occur on individual days, which are responsible for most of the
 648 mean bias and spread. On some days, the underestimation reaches more than 20 W m^{-2} .

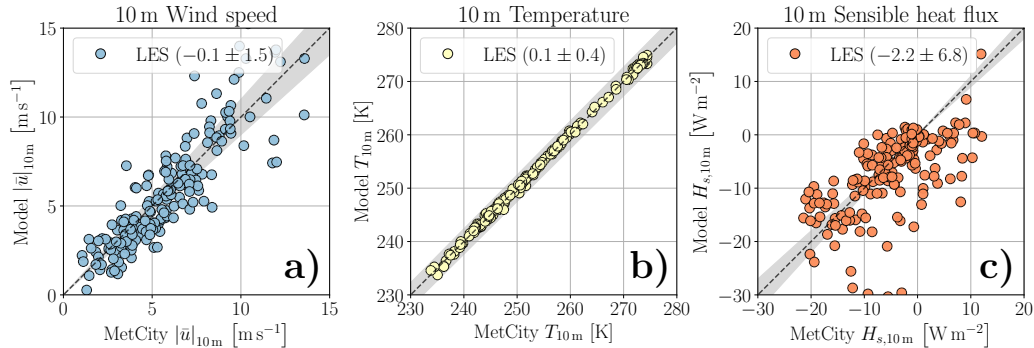


Figure 7. Scatter plots of simulated versus observed meteorological properties at 10 m height, including (a) wind speed, (b) temperature, and (c) bulk sensible heat flux. Sampling, notation, and plotting style are analogous to the previous figures.

649 The surface H_s is a key player in the SEB, an important aspect of the Arctic cli-
 650 mate system, which is crucial to correctly represent in model realizations. Accordingly,
 651 it is imperative to gain an understanding of these large differences between the model
 652 and measurements. Before claiming model shortcomings, it is relevant to first consider
 653 data comparability. At least both the model and observed fluxes rely on bulk methods.
 654 The observed fluxes were calculated using the method developed by Fairall et al. (1996),
 655 making use of turbulent transfer coefficients and roughness length estimated from the
 656 *Surface Heat Budget of the Arctic Ocean (SHEBA)* campaign (Andreas et al., 2003). For
 657 a more detailed description refer to Cox et al. (2023). As described in Section 2.2.4, the
 658 simulations also make use of stability functions based on SHEBA data (Grachev et al.,
 659 2007). But the use of roughness lengths based on daily *MOSAiC* measurements in the
 660 simulations is a key difference. Adopting the transfer coefficients and roughness lengths
 661 improved the simulations from the first attempts in terms of the H_s (not shown). How-
 662 ever, potential differences with the SHEBA roughness lengths could explain some of the
 663 remaining outlying data points.

664 More causes can be thought of to explain the differences in the H_s . These include
 665 i) local impacts on the measured fluxes not accounted for in the simulations and ii) the
 666 possible inapplicability of Monin-Obukhov similarity theory over sea ice in stable winter-
 667 tertime conditions (Heisel & Chamecki, 2023). An interesting alternative data source for
 668 comparison with the LES could be the eddy-covariance flux product that is part of the
 669 *MOSAiC* data archive (Cox et al., 2023). Further investigating these research questions
 670 is for now considered future work. The library of LES experiments presented in this study
 671 can inform this effort by providing situations for which large differences occur.

672 3.2.4 The bimodal Arctic

673 The surface energy budget of the Arctic is dominated by two primary modes. The
 674 first reflects cold, clear, and stable conditions, while the second represents warmer, cloudy
 675 states with often neutral or weakly unstable near-surface conditions. This bimodal na-
 676 ture of the Arctic climate system is a long-known phenomenon (Sverdrup, 1933) and has
 677 been measured extensively during previous drift campaigns like SHEBA (Persson et al.,

1999, 2002; Shupe & Intrieri, 2004; Stramler et al., 2011). The bimodal state has been intensely researched in recent years, given its importance in Arctic Amplification and sea ice melt. In particular, transitions between the dominant modes have been a topic of interest. Previous modeling efforts have contributed to our insight, for example, by linking the bimodality to mixed-phase cloud persistence (Morrison et al., 2012) and large-scale dynamics (Neggers, Chylík, et al., 2019). Also, well-defined bimodality has been used as a metric to test the skill of climate and single-column models (Pithan et al., 2014, 2016; Solomon et al., 2023). Because small-scale dynamics are resolved in LES instead of being parameterized, one expects a priori that the library of *MOSAIC* simulations, as discussed here, should have some skill in reproducing this feature. The availability of 190 realizations under a broad range of atmospheric conditions should provide a sufficient sample size to reproduce the bimodal distribution. These questions are addressed in this section .

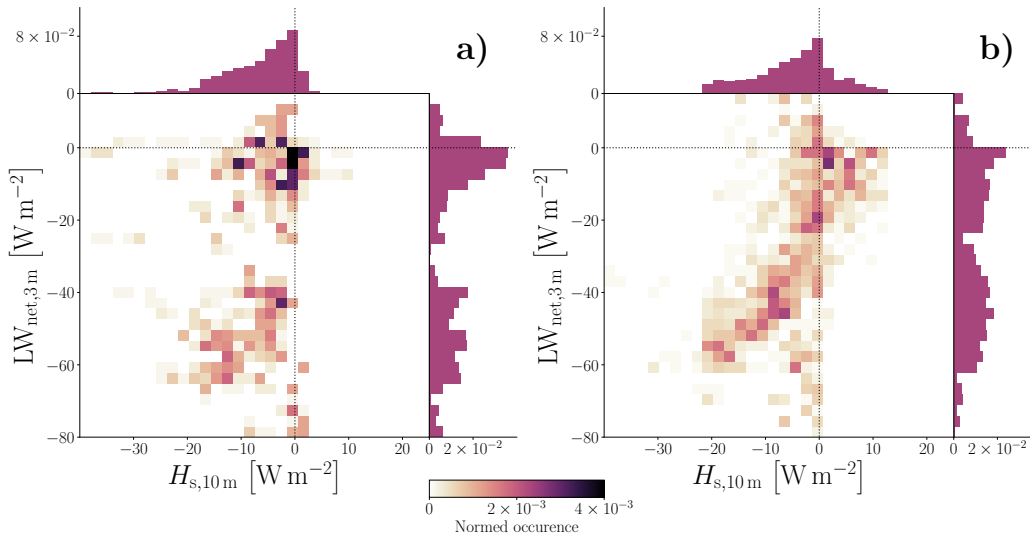


Figure 8. Two-dimensional histograms of normalized occurrence of atmospheric states characterized by the near-surface net longwave radiation (ordinate) and sensible heat flux at 10 m height (abscissa). (a) shows the LES results in which each data point of the given quantities is averaged over 15 min and the whole domain from every simulated case. (b) shows the measured values from *MetCity* (Cox et al. (2023); Fairall et al. (1996), "*bulk-Hs_10m*") between 10:45 UTC and 11:15 UTC daily.

Figure 8 shows the two-dimensional probability density function (PDF) of near-surface longwave net radiation (LW_{net}) and the near-surface sensible heat flux (H_s), as a) sampled from the year-long library of LES experiments and b) as observed during *MOSAIC*. These two variables were previously discussed individually in Sections 3.2.3 and 3.2.1, respectively, but are combined here. The bimodality is visible in the measurements, with the modes best defined along the LW_{net} axis. A variety of states is observed between the cloudy mode (near the origin) and the clear mode (bottom left). For convenience, the PDFs are also shown separately as side panels, to better determine and compare the mode locations.

For comparing the model to the measurements the two modes are now considered individually. The cloud-free mode ($LW_{\text{net}} \leq -30 \text{ W m}^{-2}$) is nearly always accompanied by a negative H_s , which can be as low as -30 W m^{-2} for extremely cold surface conditions. The model correctly reproduces this mode, although the diagonally-shaped maximum is shifted somewhat towards more negative LW_{net} values. The particularly inter-

esting cluster of cases with extremely low LW_{net} but near-zero H_s is also well captured by the model. The cloudy state ($LW_{\text{net}} > -30 \text{ W m}^{-2}$) in the LES is situated near the observed one, with a maximum occurrence of LW_{net} around 0 W m^{-2} . However, the LES fails to capture the observed weakly positive H_s occurrences and in general, is biased towards lower heat flux values (as discussed previously in Section 3.2.3). Part of a possible explanation for this underestimation could be the absence of leads in the simulations, which are known to locally boost the sensible and latent heat flux (Li et al., 2020). Additional sensitivity experiments at this location of the phase space could be informative, especially because Cox et al. (2023) note that they are likely to also miss lead effects in their bulk heat flux calculations.

A closer comparison of the simulated and observed LW_{net} side panels suggests that the LES slightly underestimates the number of intermediate states between the two dominant modes. This is also visible in the two-dimensional phase space. What causes the absence of these intermediate states in the LES is not yet fully understood, and is currently under investigation. Part of the issue could be related to the misrepresentation of longwave radiation emitted by ice clouds discussed in section 3.2.1. More possible causes include the absence of mesoscale variability in the numerical realizations due to spatially homogeneous forcing and small domain size, or an underestimation of cloud-transitional states due to characteristics of the experimental setup.

3.3 Case studies

The statistical evaluation against the full year of data in section 3.2 provides confidence in the basic skill of the LES in reproducing the cloud-radiative climate and surface energy budget of the central Arctic. This section explores a subset of three simulations in more detail. Each simulation serves as a case study of a different Arctic boundary layer, selected to accentuate results of particular interest. Table 3 gives an overview of these cases. The goal is to document resolved boundary-layer processes such as turbulence, and associated features such as vertical structure, inversions, and mixed-phase clouds. This is motivated by the potential use of these virtually resolved data sets in future research efforts.

3.3.1 Vertical structure

Figure 9 shows the potential temperature Θ , the ice q_i , liquid q_l and vapor q_v specific humidity profiles for the three cases. Analogous to previous sections, the simulations are evaluated after 1.5 h run time. The observational data sets served as initial conditions for the simulations. The value of comparing the simulation to its initial conditions is to judge how well the numerical experiment can keep the measured atmosphere in the virtual domain after the spin-up phase.

Table 3. Overview of exemplary case studies shown in section 3.3

Name	Date	Description
20191101	01 November 2019	Single layer mixed-phase cloud
20200216	16 February 2020	Mixed-phase cloud with thin ice cloud above
20200310	10 March 2020	Extremely cold icy atmosphere

The first case simulates the atmosphere measured around the *Polarstern* on November 1, 2019 at 11:00 UTC. Figure 9a-c gives an overview of the results. The boundary layer contains a well-mixed layer decoupled from the surface, as seen from the potential temperature in panel (a). The temperature inversion at 1750 m caps a mixed-phase cloud

745 seen in panel (b). It contains significant mass of liquid at the height 1200–1750 m and
 746 a minimal amount of ice at 600–1750 m. Here, the mixed-phase cloud is maintained,
 747 and the measured liquid and ice water content is reproduced. Only the ice layer around
 748 250 m measured by the ShupeTurner data sets is not found in the simulation. While tur-
 749 bulent processes intensify, the temperature and humidity profile remain nearly unchanged.
 750 Only a slight elevation and cooling of the temperature inversion is observed, as expected
 751 for a typical Arctic mixed-phase cloud.

752 The simulation for February 16, 2020 at 11:00 UTC shares several characteristics
 753 with the *20191101* case. As seen in figure 9d-f, a decoupled mixed-phase cloud is mea-
 754 sured at the *Polarstern* and reproduced by the LES. Additionally, in the spin-up time
 755 between the measurement and the evaluation of the simulation, the temperature inver-
 756 sion has lifted slightly while the cloud layer has cooled and water vapor has been depleted.
 757 In contrast to the first case, the cloud sits closer to the surface and is topped with a hu-
 758 midity inversion layer around 700 m. A clear success is the ability to maintain this hu-
 759 midity inversion right above the cloud top. The right balance between the entrainment
 760 of air above into the cloud layer and cloud-top cooling is crucial in simulating the longevity
 761 of mixed-phase clouds. The simulated liquid water profile has a maximum slightly be-
 762 low the cloud top, which is likely a more accurate profile shape than the simple adiabatic
 763 profile shape assumed in the observation-based estimate.

764 The final case discussed simulates March 10, 2020 at 11:00 UTC. It is character-
 765 ized by an extremely low boundary layer temperature, as can be seen in figure 9g. Fur-
 766 ther, panel (h) shows a significant amount of ice, especially considering the low amount
 767 of total moisture contained in the lower atmosphere (panel (i)). The large amount of ice
 768 well-distributed over the column is a typical situation for the Arctic. As discussed in sec-
 769 tion 2.3.2, ice, that is not expected to be produced by processes in turbulent clouds, is
 770 placed in the virtual domain as part of initialization. Despite the assumptions made, this
 771 simulation maintains an adequate amount of ice in the atmosphere while also depleting
 772 some of the water vapor during the 1.5 h run time. Additional research is needed to eval-
 773 uate if the model can reproduce accurate freezing rates and precipitation, as these are
 774 the main local source and sink processes for ice under extremely cold conditions.

775 **3.3.2 Mixed-phase cloud**

776 In Figure 10 the *20191101* case is shown in more detail. Panel a-c show the same
 777 vertical cross-section for the vertical velocity w , and the liquid and ice water specific hu-
 778 midities q_l and q_i . This is only one of dozens of single-layer mixed-phase clouds simu-
 779 lated in the collection of cases. In comparison to the previous discussion on the averaged
 780 vertical profiles, this figure shows the model’s capabilities in resolving the smaller-scale
 781 dynamics of mixed-phase clouds. The vertical velocity shows the up- and downdrafts in
 782 the cloud. Note, that here the downdrafts are stronger in magnitude than the updrafts,
 783 since cloud turbulence is mainly driven by cloud-top cooling. This skewness of the ver-
 784 tical velocity distribution is documented in past measurements (Shupe et al., 2013). As
 785 seen before, the typical vertical distribution of ice and liquid in mixed-phase clouds is
 786 shown: A relatively shallow liquid cloud is the source region for the formation of ice crys-
 787 tals that fall below the liquid cloud base. In this plot, the heterogeneity in the horizon-
 788 tal directions can be observed. There is a visible positive correlation between the ver-
 789 tical velocity and the liquid and ice water. Updrafts supply plentiful moisture to form
 790 and grow both cloud liquid and ice, while downdrafts entrain unsaturated air from above
 791 into the cloud. A detailed investigation of the interaction between turbulent, thermo-
 792 dynamic, radiative, and microphysical processes in Arctic mixed-phase clouds will be a
 793 future topic of research.

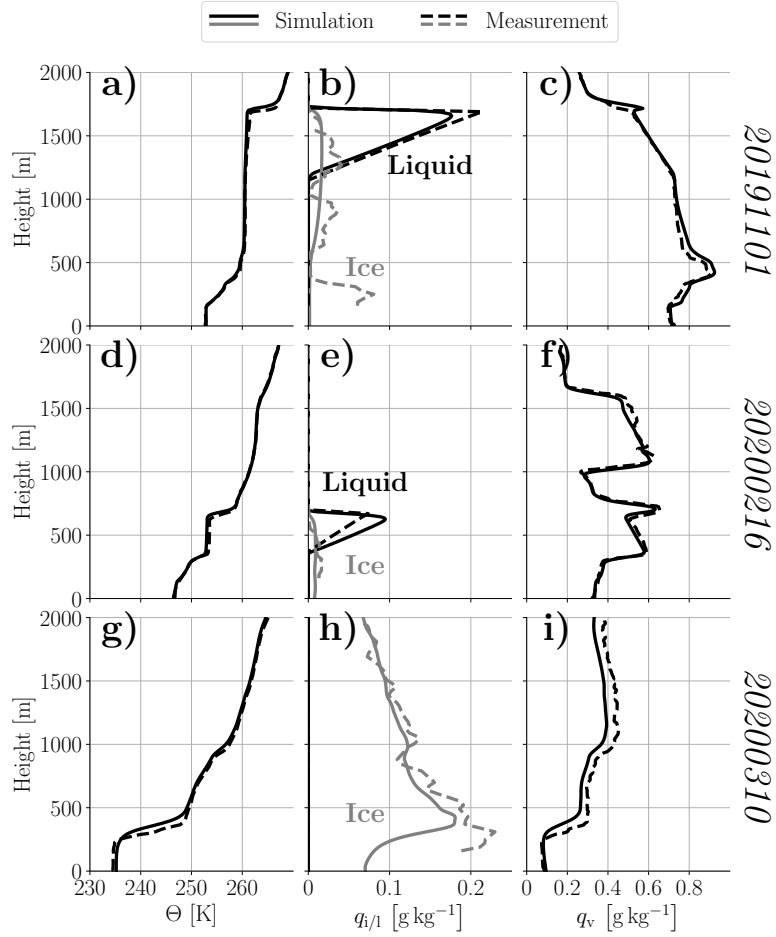


Figure 9. Analysis of the vertical profiles of potential temperature Θ , ice and water specific mixing-ratio $q_{i/l}$, and water vapor specific mixing-ratio q_v for the cases *20191101* (a-c), *20200216* (d-f) and *20200310* (g-i). Shown are the simulation results averaged over 15 min in time and over the whole domain in space after 1.5 h run time (solid) and observations at radiosonde launch time around 11:00 UTC (dashed). Observed Θ and q_v is derived from radiosonde measurements; $q_{i/l}$ is provided by the ShupeTurner data set.

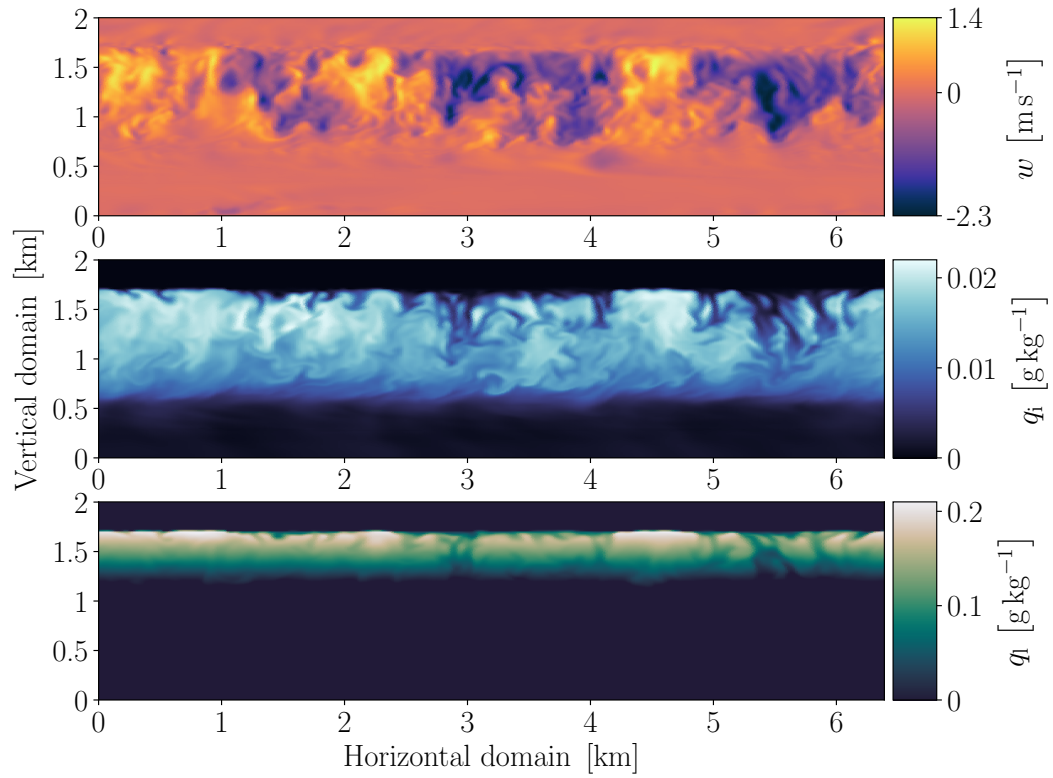


Figure 10. *20191101*: Cross-section plots of vertical velocity w , liquid specific humidity q_l and ice specific humidity q_i . The model output after 1.5 h is shown.

794 4 Discussion

795 In the creation of the year-long library of daily LES experiments, some decisions
 796 had to be made about the numerical setup, the inclusion of datasets, and the usage of
 797 various subgrid-scale parameterizations. All of these decisions affect the eventual results
 798 presented and evaluated in the previous section. Gaining insight into these impacts is
 799 part of an overarching objective of this study, which is to assess the feasibility of turbulence-
 800 resolving LES daily for long continuous periods in the Arctic theatre. To our knowledge,
 801 this has not been attempted or achieved before, and can still be considered a "terra incog-
 802 nita" (Wyngaard, 2004). In this section, the impact of various aspects is discussed in more
 803 detail to convey this experience to the scientific community and inform possible future
 804 efforts of a similar nature.

805 *Grid and domain* Existing limitations in computational resources put limits on
 806 the feasible domain size, grid size, and spatial resolution of LES. This becomes even more
 807 pressing when a high number ($\sim 10^2$) of experiments is to be performed. The first step
 808 was to adopt a vertically telescoping grid, as described in Section 2.3.1. For the PRO-
 809 Duction runs the horizontal domain size of $6.4\text{ km} \times 6.4\text{ km}$ was chosen, considered large
 810 enough to contain smaller mesoscale features but small enough to allow resolutions suf-
 811 ficient for resolving Arctic turbulence. A key step that proved crucial for arriving at an
 812 optimized setup was to use small 32×32 horizontal grid simulations for testing early
 813 versions of the model configuration. This was inspired by previous research that adopted
 814 a similar strategy for Arctic LES (Neggers, Chylík, et al., 2019). In Figure 11a this TEST
 815 setup is compared to the PRODUCTION setup in terms of downward longwave radiative
 816 flux. It is evident that the small grid TEST setup, in all its limitations, is still capable
 817 of reproducing year-average radiative climate to a high degree. This suggests good enough
 818 skill to spin up turbulence and maintain liquid clouds, which are reflected in the long-
 819 wave flux. The conclusion from this encouraging result is that using small-grid test se-
 820 tups to develop, calibrate, and optimize full LES runs in the Arctic can be effective, not
 821 just scientifically but also economically, in terms of reducing computational cost and turnover-
 822 time of numerical experiments.

823 *Representation of the surface* The representation of the surface significantly af-
 824 fects the simulations. To achieve a workable experimental setup, a few simplifications
 825 were made. First, the surface is assumed to be homogeneous, a strong simplification in
 826 a region with a notoriously heterogeneous topography (Castellani et al., 2014; Mchedlishvili
 827 et al., 2023). The sea ice surface is often covered by snow, acting as an insulator and as
 828 a source of blowing ice crystals (Wagner et al., 2022) and a variety of aerosols (Held et
 829 al., 2011; Park et al., 2019). While acknowledging these impacts, limitations in data avail-
 830 ability on these aspects motivated our decision not to represent them in the control setup.
 831 Instead, as a guiding principle, observational data was integrated on only three key sur-
 832 face variables; skin temperature, roughness, and albedo. Open-water effects are included
 833 by adapting the skin temperature and humidity to the sea-ice fraction. Figure 11b demon-
 834 strates the beneficial impact of integrating the locally observed surface skin temperature
 835 as measured at the *MetCity* site instead of using *ERA5* reanalysis data. The in-situ ob-
 836 servations are more precise in time and space for the acute situation around the *Polarstern*,
 837 and remove most of the spread introduced by the *ERA5* values. Further, the reanaly-
 838 sis values introduce a known well-defined warm bias for colder surface skin temperatures
 839 (Herrmannsdörfer et al., 2023). This is evident from the positive shift in emitted long-
 840 wave radiation for values $\leq 250\text{ W m}^{-2}$.

841 *Microphysics* In early test simulations, the default *DALES* microphysics scheme
 842 struggled to maintain liquid and frozen cloud mass for conditions below -15°C . A few
 843 microphysical processes were found to cause these issues. As described in Section 2.2.2,
 844 the parameterization for heterogeneous freezing is not valid for those temperature ranges
 845 and had to be limited to the freezing rate for conditions at -15°C . In addition, the max-
 846 imum number concentration for primary ice crystals produced by deposition-nucleation

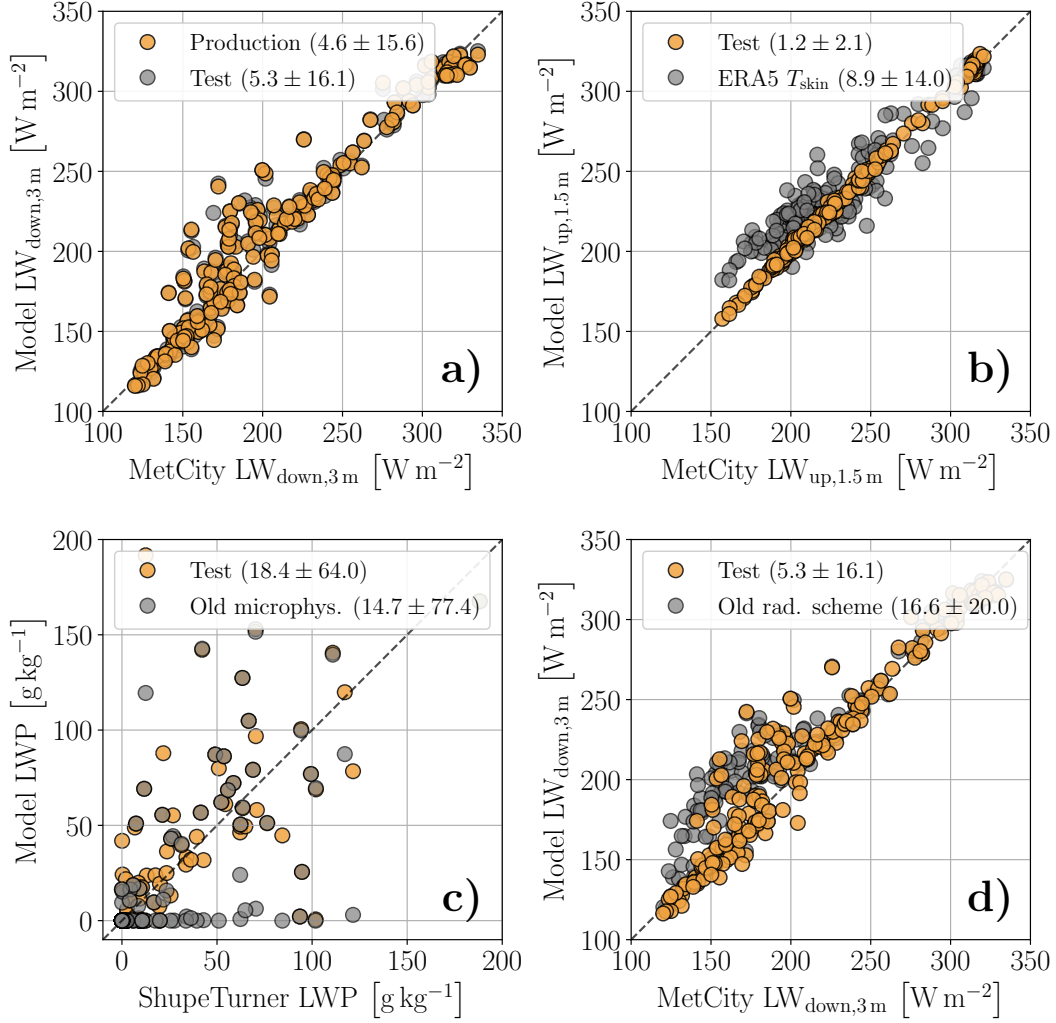


Figure 11. Scatter plots of simulated vs observed variables with different simulation setups. LES results (ordinate) are plotted against *MetCity* (Radiation) or *ShupeTurner* (LWP) measurements (abscissa). Each dot represents a single simulated daily case. The simulations are sampled at $t = 1.5$ h after initialization, the measurements are averaged for 15 min after the radiosonde launch. The dashed line indicates the one-to-one diagonal. Each panel shows the results for two different simulation setups. Panel a) shows the results in downwards longwave radiation for the PRODUCTION and the TEST setup. Analogously, panel b) shows the upwards longwave radiation for the TEST setup and a variation of it with the surface skin temperature derived from *ERA5* data. Panel c) shows the liquid water path for the TEST setup and a variation with the unchanged microphysics scheme. Panel d) shows the downwards longwave radiation for the TEST setup and a variation with the original radiation scheme.

847 is artificially limited to 200 L^{-1} . Figure 11c shows that under cold conditions, the mi-
 848 crophysics scheme in its default setting leads to a full loss of liquid for a significant sub-
 849 set of days, especially for cases with thin ice clouds measured. This loss of liquid stems
 850 from an overestimation of the ice production, quickly depleting any liquid contained in
 851 the column. Introducing the mentioned fixes in the microphysics scheme enabled real-

852 istic simulations of mixed-phase clouds throughout the year, including the Arctic win-
853 ter.

854 *Ice-radiation interaction* Another key step towards a realistic simulation of ice
855 clouds was to separate the treatment of liquid and frozen cloud mass in the radiation scheme.
856 The default *DALES* radiation scheme treated all cloud mass in the same way, a crude
857 simplification that was abandoned for the final set of runs. Figure 11d compares the near-
858 surface longwave downward radiation between the original and adjusted radiation scheme,
859 using the TEST setup. Adding separate ice-radiation interaction reduces the mean bias
860 towards higher emissions for colder atmospheres with the default scheme, in particular
861 in the presence of ice clouds, discussed in section 3.2.1. The adjustment does not com-
862 pletely remove the bias. Note, that the cause of this bias seems to stem from exceeding
863 the parameterization limits, but the cause for the large radiative effective radius of the
864 ice crystals might be twofold. Firstly, the ice crystals might be larger than the limits of
865 the radiations scheme (Ryan, 2000), but secondly, the effective radiative diameter of non-
866 spherical ice particles depends on the distribution of particle shapes (Fu & Liou, 1993;
867 Yang & Fu, 2009; Eichler et al., 2009; Mitchell et al., 2011). In 2.2.3 it is assumed that
868 the mean particle radius calculated by the bulk microphysics scheme can be used with
869 proportional ratio 1 as the radiative effective radius in the radiation scheme. The result-
870 ing bias in the longwave radiation statistics indicates that this assumption is not fully
871 correct. Improving the approximations of ice-cloud radiation emission and their depen-
872 dence on the distribution of crystal size and shapes is a goal for future research (Ham
873 et al., 2017; Cairo et al., 2023). These results suggest that the unique impact of ice clouds
874 on radiative transfer can not be ignored, and should be accounted for in model studies
875 of the Arctic climate system. This is in agreement with studies of climate models (Waliser
876 et al., 2011; Fan et al., 2023) that also conclude that further research is required to fully
877 understand and address these shortcomings (Wang et al., 2020).

878 *Other impacts* Other aspects of the experimental setup might have a significant
879 impact but are not discussed here for the sake of brevity. These include the treatment
880 of other relevant microphysical processes, aerosol, and the profiles of cloud liquid and
881 ice water content used for model initialization. Investigation of these impacts is ongo-
882 ing, making use of targeted sensitivity experiments from the library of control runs as
883 described in this study.

884 5 Summary, Conclusions and Outlook

885 This study presents a year-long library of daily high-resolution large-eddy simu-
886 lations (LES) of the atmospheric boundary layer as observed during the recent *MOSAiC*
887 drift campaign in the central Arctic. A specific target is to deeply integrate a multitude
888 of measurements into the experimental configuration. A dedicated standardized model
889 setup for Arctic conditions is developed and employed for this purpose. An overarching
890 science objective is to provide a virtual domain with resolved small-scale turbulence and
891 clouds, which can help in interpreting local measurements made at the *Polarstern* and
892 *MetCity*. To achieve the desired model skill, various sub-grid parameterizations in the
893 LES code for microphysical processes and cloud-radiative interaction had to be adapted
894 to satisfactorily work under central Arctic conditions. The production runs are statis-
895 tically evaluated against a year of *MOSAiC* data. Three individual case studies are in-
896 vestigated more closely, to assess the model’s ability to represent key boundary-layer fea-
897 tures including vertical structure and inversions, mixed-phase clouds, and turbulence.
898 The impact of various key aspects of the model and experimental setup is assessed.

899 The main scientific conclusions coming out of this research can be itemized as fol-
900 lows:

- 901 • The statistical evaluation of the library of LES runs demonstrates a generally sat-
902 isfactory performance under a broad range of meteorological conditions concern-
903 ing the surface radiative fluxes, the surface sensible heat flux, near-surface mete-
904 orology, and mixed-phase clouds.
- 905 • The bimodality in the net longwave surface flux typical of the Arctic is well re-
906 produced, with a slight underestimation of intermediate states.
- 907 • A weak overestimation of downward longwave radiation under ice clouds is iden-
908 tified, which is traced to artificial parametric limitations on the maximum effec-
909 tive diameter of ice crystals.
- 910 • Downward shortwave radiation during polar day is slightly underestimated and
911 speculated to be related to the use of one-dimensional radiative transfer in the model.
- 912 • On occasion the surface sensible heat flux, which is an interactive lower bound-
913 ary condition in the simulations, is underestimated.
- 914 • Integrating a multitude of *MOSAiC* data into the initial- and boundary conditions
915 proved crucial for achieving a good statistical agreement. This in particular ap-
916 plies to surface data, sonde data, and value-added cloud products.
- 917 • The detailed investigation of three case studies suggests that initialized liquid and
918 ice cloud layers are maintained long enough to survive in the simulations, reflect-
919 ing that cloud-radiation-turbulence interactions are well captured in this setup.
- 920 • Small grid test simulations are shown to be a viable tool for configuring and op-
921 timizing full grid LES experiments of Arctic boundary layers.

922 The obtained results, and the library of high-resolution turbulence-resolving nu-
923 merical experiments itself, create new research opportunities but also raise some new sci-
924 ence questions. An obvious new scientific opportunity is to use the simulations to gain
925 insight into Arctic Amplification at a process level. The three-dimensional model out-
926 put at high frequencies allows for the sampling of aspects of small-scale physics and dy-
927 namics that are still impossible to measure. A prime example relevant for Arctic climate
928 change is the sampling of tendencies of all terms in the energy and water budgets of the
929 Arctic boundary layer and the surface. Targeted perturbation experiments can be con-
930 ducted to test hypotheses, such as the role of small-scale physical processes in climate
931 feedback mechanisms. The first results of a boundary-layer budget analysis based on the
932 LES dataset for *MOSAiC* as presented in this study was recently published by Linke et
933 al. (2023).

934 Concerning the LES experiments, the library could still be expanded significantly;
935 only $\sim 25\%$ of radiosonde launches were used. Applying the standardized setup to gen-
936 erate more simulations at other sonde launch times is straightforward. While this would
937 represent a significant computational effort, the benefit would be an improved sample
938 size of meteorological conditions throughout the year. The range of observational data
939 sets integrated into the LES experiments could also still be expanded, which might fur-
940 ther improve model skills. In addition, for various already integrated datasets alterna-
941 tive products could be used. Assessing the impact of these actions is a future research
942 topic, and could further inform subsequent high-resolution model efforts of a similar na-
943 ture in the Arctic.

944 In this study, the model evaluation was limited to a few key *MOSAiC* datasets, se-
945 lected based on relevance but also on availability for the full drift. More such products
946 are available; in addition, a great number of special measurements are only available for
947 short intensive observation periods. These include tethered balloon data (Lonardi et al.,
948 2022; Akansu et al., 2023; Pilz et al., 2023), unmanned aerial vehicle (UAV) measure-
949 ments (Egerer et al., 2023; de Boer et al., 2022), among others. The numerical exper-
950 iments for these periods can play a role in providing context for these observational datasets
951 in terms of small-scale variability surrounding the sites. Conversely, these dedicated spe-
952 cial observations can also be used to evaluate the simulations, for example on resolved
953 processes such as turbulence, cloud microphysics, aerosol, and their interactions.

954 A significant part of the work behind this study went into deriving adequate forc-
 955 ing datasets. The content and format of these daily forcings conform to the input require-
 956 ments of most single-column models. A good example is the horizontal homogeneity of
 957 forcing profiles. With resolved LES results now available to accompany these forcings,
 958 and in combination with the extensive *MOSAiC* dataset, this creates a rich testing ground
 959 for improving larger-scale weather and climate models in the central Arctic. The option
 960 exists to test such models for both the whole drift or for a subset of days, to gain fur-
 961 ther process-level understanding and inform parameterization improvement.

962 6 Data availability

963 One of the key objectives of this work is to make all the created data available. The
 964 model code, input, and configuration, the generated forcing files, and the selected model
 965 output can be found at doi.org/10.5281/zenodo.10491362. The forcing files are compat-
 966 ible with typical single-column model (SCM) forcings because *DALES* is run with hor-
 967 izontally homogenous initial- and boundary conditions. The standard model output con-
 968 tains extensive data averaged in space and time. Some output is also available as three-
 969 dimensional fields. For a more detailed description, please refer to the accompanying doc-
 970 umentation. Additional output can always be generated. Please get in touch if needed
 971 for your research. Finally, the *DALES* version used for the final runs is 4.3 with an ex-
 972 tension for mixed-phase microphysics. The specific version used for this work is uploaded
 973 under the link above. For the official *DALES* repository please refer to <https://github.com/dalesteam/dales>.
 974 The combination of forcing files and simulation framework makes the results fully repro-
 975 ducible.

976 Appendix A Vertical grid

In this section the choice of the vertical grid is detailed. The heights of vertical lev-
 els of the grid are calculated as follows:

$$\Delta z^k = \begin{cases} \Delta z_{\text{Start}}, & \text{if } k \leq k_T \\ \Delta z_{\text{Start}} \cdot (1 + s)^{k-(k_T+1)}, & \text{if } k_M > k > k_T \\ \Delta z_{\text{End}}, & \text{if } k \geq k_M \end{cases}$$

$$z^k = \begin{cases} z^{k-1} + \Delta z^k, & \text{if } k > 1 \\ \frac{\Delta z_{\text{Start}}}{2}, & \text{if } k = 0 \end{cases}$$

$$k_T = 120, \quad s = 0.0125, \quad \Delta z_{\text{Start}} = 10 \text{ m},$$

$$k_M = 260, \quad \Delta z_{\text{End}} = 185 \text{ m}$$

977 This produces a grid with a maximum height of 11 857.23 m. The lower 1.2 km are re-
 978 solved with a fixed grid spacing of 10 m. From there, the grid spacing expands accord-
 979 ing to the given formula until it reaches $\Delta z_{\text{max}} = 185 \text{ m}$ at around 7 km height. From
 980 there the grid spacing is kept fixed again until the top of the domain. Figure A1 shows
 981 the height and grid spacing depending on the grid point.

982 Appendix B Radiosonde data

The radiosonde variables (Dahlke et al., 2023) used here are the height z , pressure
 p , temperature T , and the relative humidity RH. From these Θ_v and q_v are calculated

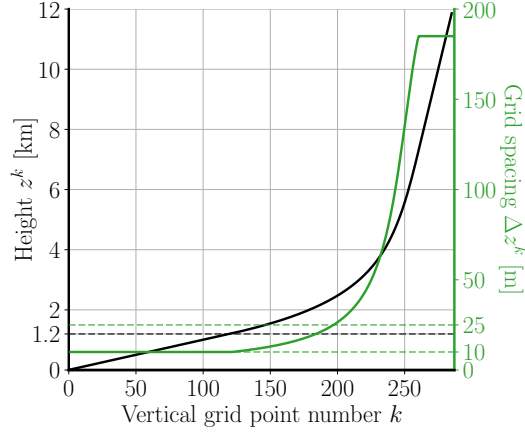


Figure A1. Vertical grid height and spacing of the standardized simulation setup.

using Tetens formula (Tetens, 1930; Murray, 1967):

$$\Theta = T \cdot (p_{\text{ref}}/p)^{R_d/c_p} \quad (\text{B1})$$

$$e_{\text{sat},l} = e_{\text{sat},0} \cdot \exp [a_t \cdot (T - T_m)/(T - b_t)] \quad (\text{B2})$$

$$q_{\text{sat},l} = \frac{R_d/R_v \cdot e_{\text{sat},l}}{p - (1 - R_d/R_v) \cdot e_{\text{sat},l}} \quad (\text{B3})$$

$$q_v = \text{RH} \cdot q_{\text{sat},l} \quad (\text{B4})$$

$$\Theta_v = \Theta \cdot (1 + 0.61 \cdot q_v) \quad (\text{B5})$$

983 Here, $a_t = 17.27$ (dimensionless) and $b_t = 35.86$ K are dimensionless parameteriza-
 984 tion constants, $e_{\text{sat},0} = 610.78$ Pa the reference vapor pressure constant, $R_d = 287.04$ J kg⁻¹ K⁻¹
 985 and $R_v = 461.5$ J kg⁻¹ K⁻¹ the gas constants for dry air and water vapor, $c_p = 1004$ J kg⁻¹ K⁻¹
 986 the specific heat capacity, $T_m = 273.16$ K the melting temperature of ice and $p_{\text{ref}} =$
 987 1000 hPa the reference pressure. Θ is the potential temperature, e_{sat} the saturation wa-
 988 ter vapor pressure with respect to liquid and q_{sat} the corresponding saturation specific
 989 humidity.

A further correction to the derived sonde water vapor specific humidity (q_v) pro-
 file is made: Thin, high-level ice clouds frequently occur in the Arctic atmosphere - in
 areas where the air is saturated with water vapor concerning ice. Small measurement
 uncertainties can lead to situations where $q_v > q_{\text{sat},i}$ and therefore place unrealistic amounts
 of cloud ice in the simulation domain. This is prevented by setting

$$q_v(z) = \min [q_{\text{sat},i}(z), q_v(z)], \quad \text{for } z \geq z_{\text{cut}} \quad (\text{B6})$$

Here, $q_{\text{sat},i}$ is the saturation vapor pressure concerning ice calculated analogously to equa-
 tion (B2) and (B3) with $a_{t,i} = 21.8746$ and $b_{t,i} = 7.66$ K. The cutoff length z_{cut} is cho-
 sen to divide the vertical domain into areas of turbulent ice production in the bound-
 ary layer (e.g., in mixed-phase clouds) and areas of deposition ice production. It is cal-
 culated as the layer of the highest occurring liquid water content q_l above a threshold:

$$z_{\text{cut}} = \max_z \{z \mid q_l(z) \geq 0.01 \text{ g kg}^{-1}\} \quad (\text{B7})$$

990 Here, q_l is derived as described in section 2.3.2.

991 Appendix C Evaluation point

992 To ensure comparability between all cases, a common point in time to evaluate the
 993 simulations has to be found. Different issues have to be considered: First, the grand goal

994 of this work is to be able to compare the simulations to *MOSAIC* measurements. The
 995 initial conditions are derived once at the start of the simulation and, besides weak nudg-
 996 ing, do not influence the further evolution of the atmosphere in the virtual domain. Nat-
 997 urally, after some time, the conditions will have changed so much due to internal tur-
 998 bulent, radiative, and microphysical processes that there is no value in comparing the
 999 LES to the measurements anymore. This motivates an early time point for evaluation.
 1000 But, it has to be considered that the simulation needs time to "spin up". Initially, all
 1001 variables in the LES are homogeneously distributed in the horizontal directions. Their
 1002 vertical distribution and wind lead to turbulent mixing in the domain, ultimately creat-
 1003 ing a realistic spatial distribution of the prognostic variables.

1004 Quantifying the right point in time, considering both of these issues, is difficult to
 1005 achieve since the atmospheric state varies strongly from case to case. Figure C1 shows
 1006 the distribution of the absolute change in total turbulent kinetic energy (TKE) in the
 1007 collection of cases dependent on time. For better comparison, the values are normalized
 1008 by the average value in the shown interval. Generally speaking, the spin-up phase is as-
 1009 sociated with a quick change in TKE, since turbulent processes are still developing. A
 1010 small change in TKE signifies a period of quasi-equilibrium, where the state of the at-
 1011 mosphere is not shifting significantly. Therefore, the point in time for the evaluation of
 1012 the simulations is chosen to be 1.5 h, around the general minimum of change in TKE.

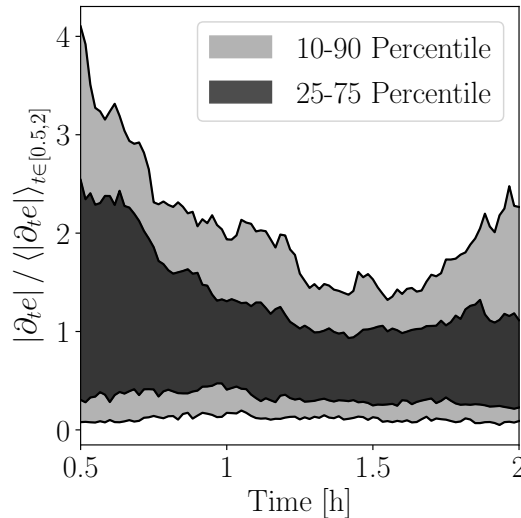


Figure C1. Distribution of normalized absolute change in total turbulent kinetic energy of all simulated cases depending on simulation time.

1013

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1 **Standardized daily high-resolution large-eddy**
2 **simulations of the Arctic boundary layer and clouds**
3 **during the complete *MOSAIC* drift**

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8 **Key Points:**

- 9 • Campaign data is deeply integrated into the experimental design of daily turbulence-
10 and cloud-resolving simulations.
- 11 • Independent drift-long statistics on key aspects of the surface energy budget, ther-
12 modynamic structure, and clouds are reproduced.
- 13 • Sensitivities of the results to the experimental design and model physics are ex-
14 plored.

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Abstract

This study utilizes the wealth of observational data collected during the recent *MOSAiC* drift experiment to constrain and evaluate 190 daily Large-Eddy Simulations (LES) of Arctic boundary layers and clouds at turbulence-resolving resolutions. A standardized approach is adopted to tightly integrate field measurements into the experimental configuration. Covering the full drift represents a step forward from single-case LES studies, and allows for a robust assessment of model performance against independent data under a broad range of atmospheric conditions. A homogeneously forced Eulerian domain is simulated, initialized with radiosonde and value-added cloud profiles. Prescribed boundary conditions include various measured surface characteristics. Time-constant composite forcing is applied, primarily consisting of subsidence rates sampled from reanalysis data. The simulations run for multiple hours, allowing turbulence and mixed-phase clouds to spin up while still facilitating direct comparison to *MOSAiC* data. Key aspects such as the vertical thermodynamic structure, cloud properties, and surface energy fluxes are satisfactorily reproduced and maintained. Specifically, the model captures the bimodal distribution of atmospheric states that is typical of Arctic climate. Selected days are investigated more closely to assess the model's skill in maintaining the observed boundary layer structure. The sensitivity to various aspects of the experimental configuration and model physics is tested. The model input and output are available to the scientific community, supplementing the *MOSAiC* data archive. The close agreement with observed meteorology justifies the use of LES data for gaining further insight into Arctic processes and their role in Arctic climate change.

Plain Language Summary

The Arctic is one of the regions most affected by global climate change, warming up to four times as fast as the rest of the globe. It is also a particularly inaccessible region to conduct measurements. Fortunately, between 2019 and 2020 the *MOSAiC* campaign collected an unprecedented amount of data in the Arctic. In this study, numerous of these measurements are incorporated into high-resolution computer simulations of the lowest part of the Arctic atmosphere. This simulation data complements and contextualizes the observations and enables insight into complex physical processes, e.g., cloud formation, ice production, or turbulent mixing. The Arctic is an extreme place, and models often struggle to represent the atmosphere accurately. Therefore, the main achievement of this study is to successfully simulate 190 atmospheric situations as measured during the campaign. The generated data set performs well when compared to independent observations. Single cases deliver information about individual atmospheric conditions, and the collection gives insight into how key climate variables behaved throughout the *MOSAiC* year.

1 Introduction

The ongoing rapid warming of the Arctic region is a significant contributor to global climate change. Due to amplification processes, the Arctic warms up to four times as fast as the rest of the globe (Serreze & Barry, 2011; Rantanen et al., 2022). Past research suggests various feedback processes cause this Arctic Amplification (AA) (Wendisch et al., 2023), including the albedo (Screen & Simmonds, 2010; Thackeray & Hall, 2019; Dai et al., 2019; Jenkins & Dai, 2021), Planck (Pithan & Mauritsen, 2014), water-vapor, lapse rate (Stuecker et al., 2018; Linke et al., 2023), and cloud feedback (Philipp et al., 2020; Middlemas et al., 2020). To better understand these feedback mechanisms, it is crucial to quantify the effects of turbulent boundary layer processes in the Arctic atmosphere amid a changing climate (Taylor et al., 2018). Furthermore, it is essential to inform large-scale model parameterizations with high-resolution modeling efforts. Here, a collection of 190 of these numerical experiments is created by integrating a variety of Arctic measurements.

The investigation of the high Arctic is highly challenging for various reasons. The dynamic sea-ice masses make it impossible to install permanent measuring stations. Therefore, reliable meteorological data from ship- and airborne measurement campaigns and satellite imagery is sparsely available. All of which suffer from spatial and temporal gaps in the coverage. The *Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC, Shupe et al. (2020))* was a major international field campaign that took place in the Arctic from September 2019 to October 2020, intending to fill essential data gaps in in-situ observations in the central Arctic, covering an entire annual cycle. The campaign involved the deployment of the German research vessel *Polarstern*, which was frozen into the Arctic sea ice and drifted with it for over a year. During this time, the campaign and connected projects gathered an unprecedented amount of highly diverse data sets and made them available to the research communities in atmospheric, cryospheric, and oceanic sciences (Shupe et al., 2022; Nicolaus et al., 2022; Rabe et al., 2022).

The first objective of this work is to integrate available observational data sets from the *MOSAiC* campaign into a high-resolution numerical experiment. This supplements the data record with time-resolved three-dimensional modeling results and augments singular data sets by contextualizing their role in a turbulent boundary layer. A quantity of high-resolution Large Eddy Simulations (LES) are performed to achieve this.

LES is valuable for resolving critical small-scale boundary layer processes, including cloud dynamics and turbulence. This method also employs well-established parameterization techniques for surface energy exchange and micro-physical processes to facilitate the simulation of larger domains, allowing for the formation of mesoscale structures. LES has been extensively utilized in boundary layer research for several decades - also in the Arctic region. Granted, past model intercomparison studies show weaknesses and strong sensitivities in representing (mixed-phase) cloud properties (Klein et al., 2009; Fridlind et al., 2012; Ovchinnikov et al., 2014; Stevens et al., 2018) and there is strong evidence suggesting a high spatial resolution is needed to accurately represent the turbulent dynamics in a rather energy-sparse Arctic atmosphere (van der Linden et al., 2020; van der Linden & Ansorge, 2022). Nonetheless, there have been several additional successful studies using LES for Arctic boundary layer research (e.g., Solomon et al. (2011); Morrison et al. (2011); Neggers, Chylik, et al. (2019); Egerer et al. (2021); Chylik et al. (2023)): This demonstrates the importance of a careful setup to achieve an accurate representation of the Arctic atmosphere in a virtual domain. The amount of *MOSAiC* datasets enables a setup with a minimum of uncertainties as well as a fair and thorough evaluation of the results.

The overarching goal of this particular work is to create a suit of 190 high-resolution LES representing the conditions of the lower Arctic atmosphere throughout the whole *MOSAiC* year. The choice of days was purely taken based on sufficient data availability. This approach has two main objectives: First, learn about the Arctic climate system, especially smaller-scale processes that are difficult to measure reliably and can hardly be accurately represented in larger-scale models. Second, identify weaknesses in the model

107 under different conditions by evaluating the simulation results against a large amount
 108 of diverse *MOSAiC* data sets. Therefore, keeping a standardized setup for each case is
 109 crucial to discovering systematic framework or parameterization problems. Initial and
 110 boundary conditions, model settings, and evaluation are all done without any manual
 111 adjustment on a case-to-case basis. The approach taken in this work sets it apart from
 112 individual case studies that prioritize optimizing single simulations at the expense of gain-
 113 ing a broader understanding of the model’s potential weaknesses, which a highly customized
 114 configuration may mask. It also enables the creation of impact studies for a diverse li-
 115 brary of cases by modifying this standardized setup.

116 The idea of standardized multi-month/multi-year LES has been successfully em-
 117 ployed at different super-sites where continuous data is available, e.g., at Cabauw, Nether-
 118 land (Neggers et al., 2012; Schalkwijk et al., 2015), at JOYCE, Germany (van Laar et
 119 al., 2019), within the LASSO project (Gustafson Jr et al., 2020) or even in more north-
 120 ern places as Svalbard (Kiszler et al., 2023). The *Polarstern* and the surrounding mea-
 121 surement stations act as a one-year super-site.

122 Section 2 gives a detailed description of the method, including an overview of the
 123 datasets used, the numerical model framework, and the configuration of the experiments
 124 based on the *MOSAiC* data. The results of the simulation and their evaluation against
 125 measurements are presented in section 3. A detailed discussion of the results’ meaning,
 126 implications, and limitations is found in section 4. Finally, section 5 summarizes the main
 127 conclusions of this study and provides an outlook on future research it might inspire.

128 2 Data and Method

129 2.1 *MOSAiC* datasets

130 At the foundation of the drift-covering library of high-resolution Large Eddy Sim-
 131 ulations of the Arctic atmospheric boundary layer discussed in this study are the obser-
 132 vational datasets collected during the *MOSAiC* drift. Table 1 gives a complete overview
 133 of these data. It includes the variable, its units and full name, the dimensionality, the
 134 associated instrument, and the scientific study presenting the dataset. We refer to these
 135 publications for a more detailed technical and scientific description of these datasets and
 136 the associated instruments.

137 Vertical profiles of the thermodynamic state, including temperature and water va-
 138 por specific humidity, are provided by the daily 11:00 UTC radiosonde launches during
 139 the *MOSAiC* campaign (Maturilli et al., 2022; Dahlke et al., 2023). Vertical cloud liq-
 140 uid and ice water content profiles are obtained from the value-added cloud product based
 141 on remote sensing datasets as described by Shupe et al. (2015). Information on cloud
 142 condensation nuclei concentrations is based on aerosol measurements (Koontz et al., 2020),
 143 while ice nucleating particle concentrations are based on the aerosol measurements by
 144 Creamean (2022). The skin temperature of the sea ice is based on the brightness tem-
 145 perature measurements from the *MetCity* location on the sea ice (Cox et al., 2023; Cox
 146 et al., 2023). Also based on tower measurements are estimates of the surface aerodynamic
 147 roughness length (Gallagher, 2023). Finally, surface albedo values are obtained from satel-
 148 lite products (Spreen et al., 2008; Istomina et al., 2020).

149 A few datasets required for the configuration of the daily numerical experiments
 150 are not mentioned in Table 1 because they are based on *ERA5* reanalysis data (Hersbach
 151 et al., 2018a, 2018b, 2023). These include vertical profiles of horizontal wind and time
 152 series of the sea-ice fraction. The motivation for using reanalysis products for these vari-
 153 ables is to make the simulated domain reflect a larger area and avoid introducing ultra-
 154 local effects. A few variables are also derived from *ERA5* because they were not mea-
 155 sured during the *MOSAiC* drift. These include large-scale vertical motion (subsidence)

156 and pressure gradients, adopting the procedure implemented by Neggers, Chylik, et al.
157 (2019); van Laar et al. (2019).

158 The resulting simulations are evaluated against additional *MOSAIC* datasets in-
159 dependent from those used in the experimental design. Simulated short- and longwave
160 radiative fluxes are compared to sensor data of the radiation station described by Cox
161 et al. (2023) and Riihimaki (2021). This installation was part of *MetCity* with sensors
162 placed at 3 m (upwelling) and 1.5 m (downwelling) height. Simulated near-surface tur-
163 bulent heat fluxes are evaluated against data described by Cox et al. (2023), who dis-
164 cuss two different heat flux datasets. One is directly retrieved from sonic-anemometer
165 turbulence measurements, while the other is a bulk calculation based on Monin-Obukhov
166 theory. The latter is used in this study, although Cox et al. (2023) do mention poten-
167 tial over-simplifications, such as the assumption of constant roughness lengths. Since the
168 surface flux parameterization in the model is also based on Monin-Obukhov theory, the
169 use of bulk measurements yields the fairest comparison of the model to data.

170 2.2 Model setup

171 2.2.1 *LES* code

172 The *Dutch Large Eddy Simulation* framework (*DALES*, Heus et al. (2010)) was uti-
173 lized in this research. This code has been effectively employed in numerous boundary
174 layer studies (de Roode et al., 2016; Van der Dussen et al., 2013; van Laar et al., 2019),
175 particularly also to conduct Arctic research (Neggers, Chylik, et al., 2019; de Roode et
176 al., 2019; Chylik et al., 2023; Egerer et al., 2021). The foundation of the model is the
177 Ogura-Phillips anelastic equations for a set of prognostic variables, including liquid wa-
178 ter potential temperature Θ_1 , the velocity components $\{u, v, w\}$, total water specific hu-
179 midity q_t , and the mass concentration as well as number concentration of various hydrom-
180 eteor species. Momentum advection is calculated by a fifth-order central difference scheme
181 and scalar advection by a κ -limiter scheme (Hundsdoerfer et al., 1995). A prognostic TKE
182 model calculates the subgrid-scale transport of heat, moisture, and momentum. Finally,
183 the time integration makes use of a 3rd-order Runge-Kutta scheme. To better represent
184 mixed-phase clouds in a wide range of conditions, we enhanced the cloud microphysics
185 scheme, the radiation scheme, and the surface scheme, as described in more detail be-
186 low.

187 2.2.2 *Microphysics*

188 The mixed-phase, double-moment micro-physics scheme by Seifert and Beheng (2006)
189 has enabled the inclusion of ice-cloud processes in investigations of the Arctic climate
190 system and has been used in various research projects and models (Schemann & Ebell,
191 2020; Kiszler et al., 2023; Chylik et al., 2023; Linke et al., 2023). It considers the mass
192 and number concentration of five hydro-meteors: Cloud droplets and cloud ice crystals
193 and the precipitating hydro-meteors snow, graupel, and rain. The cloud condensation
194 nuclei concentration is single-species and prognostic, while the ice nucleating particle con-
195 centration is also single-species but prescribed, and its activation depends on temper-
196 ature. The microphysics scheme was initially designed for simulating ice clouds in the
197 mid-latitudes and, therefore, requires evaluation and partial adaptation to suit the ex-
198 tremely cold conditions in the high Arctic. Two key changes to the original implemen-
199 tation (Chylik et al., 2023) were made: Firstly, we calculate the heterogeneous freezing
200 rates using the maximum of the actual atmospheric temperature and $T_{\text{het,lim}} = -15^\circ\text{C}$,
201 as temperatures below this threshold lead to the edges of the valid range of the param-
202 eterization being approached and exceeded (Pruppacher & Klett, 1996). Secondly, the
203 maximum number concentration of nucleated ice particles produced by deposition-nucleation
204 is limited to $c_{N,\text{ice}} = 200 \text{ L}^{-1}$ to prevent an unrealistically high concentration of tiny
205 ice particles, which would exceed the estimated concentration of available ice nucleat-

Table 1. Overview of observational data sets utilized to set, constrain, and evaluate the conducted simulations.

Variable	Unit	Description	Dimension	Instrument	Citation
α	%	Surface albedo	(t)	AMSR-E Satellite	Spreen et al. (2008); Istomina et al. (2020)
q_v	kg kg^{-1}	Water vapor specific humidity	(z, t)	Radiosonde	Maturilli et al. (2022); Dahlke et al. (2023)
Θ_v	K	Virtual potential temperature	(z, t)	Radiosonde	Maturilli et al. (2022); Dahlke et al. (2023)
q_l	kg kg^{-1}	Liquid water specific humidity	(z, t)	Multi-sensor retrieval	Shupe et al. (2015)
q_i	kg kg^{-1}	Ice water specific humidity	(z, t)	Multi-sensor retrieval	Shupe et al. (2015)
LW_d	W m^{-2}	Longwave downward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
LW_u	W m^{-2}	Longwave upward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
SW_d	W m^{-2}	Shortwave downward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
SW_u	W m^{-2}	Shortwave upward radiative flux	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
T_{skin}	K	Skin temperature	(t)	Radiation station	Cox et al. (2023); Riihimaki (2021)
$U_{10\text{m}}$	m s^{-1}	10 m wind speed	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$T_{10\text{m}}$	K	10 m temperature	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$H_{s,10\text{m},\text{bulk}}$	W m^{-2}	10 m Bulk sensible heat flux	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$H_{s,10\text{m},\text{turb}}$	W m^{-2}	10 m Turbulent sensible heat flux	(t)	Meteorological tower	Cox et al. (2023); Cox et al. (2023)
$z_{0,m}$	m	Roughness length for momentum	(t)	Meteorological tower	Cox et al. (2023); Gallagher (2023)
c_{CCN}	m^{-3}	Cloud condensation nuclei concentration	(t)	ARM optical particle counter	Koontz et al. (2020)
c_{INP}	m^{-3}	Ice nucleating particle concentration	(t)	DRUM aerosol sampler	Creamean (2022)

206 ing particles. However, these limits do not apply to the secondary production of ice. It
 207 is worth noting that developing an accurate microphysics scheme for the Arctic is a highly
 208 researched topic (Fridlind et al., 2012; Ong et al., 2022) that cannot be covered within
 209 the scope of this study, but by including the mentioned changes, realistic ice production
 210 has been achieved.

211 **2.2.3 Radiation**

212 By default, *DALES* uses a four-stream solver based on (Fu & Liou, 1993; Liou et
 213 al., 1988) in combination with Monte Carlo Spectral Integration (Pincus & Stevens, 2009)
 214 to calculate the vertical component of the radiative fluxes in the short- and longwave.
 215 Previously, the optical properties of ice water content in the radiation calculation were
 216 estimated to be identical to a liquid water content of the same mass and a prescribed
 217 constant number concentration. While this was expected to introduce an inevitable er-
 218 ror in general, it proved to be an unusable assumption for thin ice clouds in the Arctic.
 219 For this work, the description of the optical properties of ice crystals followed Fu and
 220 Liou (1993). This parameterization was developed for cirrus ice clouds with effective ice
 221 diameter in the range 20 – 120 μm .

222 Prior to this study the *DALES* code had never been applied to central Arctic con-
 223 ditions. A necessary step was to supply the radiation scheme with realistic information
 224 about the effective diameter of ice crystals. These are here based on the physical prop-
 225 erties of ice crystals (McFarquhar & Heymsfield, 1998; Baran, 2005), as estimated from
 226 the microphysics scheme. How microphysical properties of ice crystals such as size, ge-
 227 ometry, and density can be linked to radiative properties is not yet fully understood, and
 228 is an active research topic (Ryan, 2000; Mitchell, 2002; Konoshonkin et al., 2017; Ham
 229 et al., 2017). For this reason, the mean particle diameter calculated by the microphysics
 230 bulk scheme is for simplicity directly used as the radiative effective diameter. This sim-
 231 plification should be kept in mind when interpreting the results presented in this study.
 232 Testing more complex models for the effective diameter of ice particles in the LES is for
 233 now considered a future research topic.

234 Finally, two further simplifications in the treatment of radiation should be men-
 235 tioned. Firstly, in grid boxes with a mean ice crystal size outside of the range defined
 236 above, the effective diameter is set to the upper (respectively lower) bound. Secondly,
 237 the solar zenith angle is set constant for the duration of each simulation, and is calcu-
 238 lated based on the location and time of the radiosonde used for initialization of the model.
 239 The zenith angle affects the solar radiation, but three-dimensional effects are not con-
 240 sidered, and radiative transfer works purely in the vertical.

241 **2.2.4 Surface parameterization**

The parameterization of surface processes, particularly flux calculations, becomes
 necessary when using *DALES* due to the unresolved surface-roughness scale. Assuming
 that the first model level lies in the atmospheric surface layer, computing the exchange
 between atmosphere and surface becomes possible based on the Monin-Obukhov theory
 and the surface layer bulk Richardson number Ri_B (Louis, 1979):

$$242 \quad Ri_B = \frac{z_1}{L} \frac{\left[\ln \frac{z_1}{z_{0,h}} - \Psi_H \left(\frac{z_1}{L} \right) + \Psi_H \left(\frac{z_{0,h}}{L} \right) \right]}{\left[\ln \frac{z_1}{z_{0,m}} - \Psi_M \left(\frac{z_1}{L} \right) + \Psi_M \left(\frac{z_{0,m}}{L} \right) \right]^2}. \quad (1)$$

243 Here, z_1 is the height of the first model level, L the Obukhov length, $z_{0,h}$ and $z_{0,m}$ the
 244 roughness lengths for heat and momentum, respectively, and Ψ_H and Ψ_M the integrated
 245 stability functions. For a more detailed description refer to Heus et al. (2010).

246 The stability functions for the unstable and neutral conditions are unchanged from
 the initially released code base, while for the stable conditions, the stability functions

247 by Grachev et al. (2007) are newly implemented. They were specifically developed for
 248 the Arctic regime based on data from the SHEBA campaign suiting this application. The
 249 use of roughness lengths derived from MOSAiC measurements is discussed in section 2.3.4.

250 Originally, the computation of sensible and latent heat fluxes at the surface relied
 251 on a single uniform surface skin temperature. However, a slightly different approach was
 252 introduced, which considers two distinct skin temperatures: the ice skin temperature mea-
 253 sured and the ocean skin temperature set to $t_{\text{skin,ocean}} = -1.8^\circ\text{C}$. By computing fluxes
 254 for both temperatures and then taking a weighted average based on the sea-ice fraction,
 255 this approach allows for partial inclusion of open ice effects into the simulation. If the
 256 ice temperature exceeded -1.8°C , ocean and sea-ice temperature were assumed to be
 257 identical.

258 The ice skin temperature is prescribed and constant throughout the simulation. This
 259 one-way surface-atmosphere coupling reduces the complexity of the simulation immensely,
 260 and the error it introduces is expected to be minimal, primarily because of relatively short
 261 simulation times.

262 **2.3 Experimental configuration**

263 **2.3.1 Domain and grid**

The choice of domain and grid size is crucial for the quality of a simulation. The
 adopted spatial discretization reflects the limits computational resources impose on sim-
 ulating a full year at turbulence-resolving resolutions. Ensuring that turbulent structures
 are accurately represented is imperative, which requires a sufficient grid resolution. To
 avoid the unwanted effects of periodic boundaries in the horizontal directions, the do-
 main must be appropriately sized to provide mesoscale structures with enough space to
 evolve. In the standardized setup, the horizontal domain and grid utilized are:

$$L_x = L_y = 6400 \text{ m}$$

$$\Delta x = \Delta y = 20 \text{ m}$$

264 An Eulerian framework is adopted, with the domain fixed in space at the *Polarstern* lo-
 265 cation. This choice is motivated by our double objective of i) performing short-range sim-
 266 ulations lasting only a few hours and ii) being able to compare model results to station-
 267 ary measurements.

268 The top of the vertical domain is at $L_z \approx 12 \text{ km}$. The lowest 1200 m of the field
 269 is resolved with a grid spacing of $\Delta z_{\text{min}} = 10 \text{ m}$. Above this level, the grid spacing in-
 270 creases exponentially with height until a maximum grid spacing of $\Delta z_{\text{max}} = 185 \text{ m}$. The
 271 non-regular vertical grid allows for high resolution in the cloud-containing boundary layer
 272 while also accommodating tropospheric features such as higher-level clouds that primar-
 273 ily exert radiative effects on the lower domain. In total, the grid consists of 286 verti-
 274 cal levels. For a more detailed description refer to Appendix A

275 In the process of finding a compromise between domain size and resolution with
 276 fixed available computational resources, it was decided to prioritize resolution: The $6.4 \text{ km} \times$
 277 6.4 km domain is enough to allow for thermodynamic heterogeneities in the virtual area
 278 but might lack the evolution of larger mesoscale structures. Since this work is focused
 279 on accurately representing realistic conditions and smaller-scale processes in the Arctic
 280 atmospheric boundary layer, the resolution that has been selected is satisfactory. The
 281 small grid boxes, especially in the lowest layers, enable an accurate representation of tur-
 282 bulance and all turbulence-driven processes, e.g., cloud evolution and life cycle, entrain-
 283 ment, shear-layer mixing, detailed distribution of microphysical interactions, surface fluxes,
 284 etc. This setup is referred to as PRODUCTION setup in the following.

285 A second configuration (TEST) was employed: By reducing the horizontal domain
 286 to $800 \text{ m} \times 800 \text{ m}$ and the horizontal resolution to $25 \text{ m} \times 25 \text{ m}$ the computational ex-
 287 pense is reduced drastically. The vertical grid is kept unchanged. While this resolution
 288 and domain size decrease the simulation quality, the results are still greatly informative.
 289 The TEST configuration proved to be crucial in curating and testing the standardized

290 setup and the integration of measurements in an efficient manner. This procedure of us-
 291 ing micro-grids to inform the setup of expensive runs was inspired by Neggers, Chylik,
 292 et al. (2019). Table 2 summarizes the two setups.

Table 2. Resolution and domain size for different setups.

Setup	Resolution (h × v)	Domain (h × v)	Usage
PRODUCTION	20 m × (10 – 185 m)	6.4 km × 12 km	Definitive runs
TEST	25 m × (10 – 185 m)	0.8 km × 12 km	Impact studies

293 **2.3.2 Initial profiles**

294 The initial conditions of each simulation are mostly derived from data gathered dur-
 295 ing the *MOSAIC* campaign to constrain the experiments as much as possible with mea-
 296 surements. All initial profiles, most of which concern prognostic variables in the model,
 297 are horizontally homogeneous in the simulation domain.

298 Initial profiles of the two prognostic thermodynamical state variables in *DALES*,
 299 total water specific humidity q_t and liquid water potential temperature θ_l , are derived
 300 from data from the 11:00 UTC radiosonde launched at the *Polarstern* (Maturilli et al.,
 301 2022). Corrections were applied to account for elevated launch height and initial sen-
 302 sor adjustment after launch by Dahlke et al. (2023). For this purpose, the radiosonde
 303 data was combined with measurements from the *MetCity* meteorological tower (Cox et
 304 al., 2023). The prognostic model variables q_t and θ_l in the *DALES* code are derived from
 305 the radiosonde temperature, humidity, and pressure measurements. Further, for ice lay-
 306 ers, the derived q_v profile was bounded by the saturation specific humidity $q_{sat,i}$, to limit
 307 the impact of measurement uncertainties on the sensitive initialization of ice clouds. The
 308 full procedure is detailed in Appendix B.

309 The two prognostic variables of suspended cloud mass, cloud liquid water content
 310 (LWC) and ice water content (IWC), are also initialized with measurement-based pro-
 311 files. In the *DALES* code, these variables are denoted as q_l and q_i , respectively. Initial-
 312 izing cloud variables with observations reflects our objective of simulating and resolv-
 313 ing small-scale turbulent variability around the *MOSAIC* instrumentation, which is of-
 314 ten driven by cloud processes. One could initialize with a cloud-free state and let mixed-
 315 phase clouds develop by themselves over time. However, previous LES intercomparison
 316 studies on mixed-phase clouds have shown that this is difficult to achieve in a short sim-
 317 ulation time (Neggers, Chylik, et al., 2019; Stevens et al., 2018), and the simulations tend
 318 to drift significantly away from the initialized atmospheric thermodynamic state as the
 319 clouds form. These points motivated the adoption of direct initialization of cloud mass.
 320 To achieve this, accurate placement and phasing of the initial cloud mass relative to the
 321 vertical atmospheric thermodynamic profile is imperative. Because cloud mass is not di-
 322 rectly measured by the radiosonde, the data product of Shupe et al. (2015) is used in this
 323 study. The multi-sensor cloud retrieval product features vertically resolved LWC and IWC
 324 at 1 min resolution. To ensure that extreme values are avoided and the overall thermo-
 325 dynamic state of the boundary layer is captured, the initial conditions used are mean
 326 LWC and IWC profiles. This approach focuses on representing the average conditions
 327 across the entire domain rather than the potential heterogeneities in certain areas. In
 328 each case, the 1 min profiles from the data set are averaged for 15 min after the radiosonde
 329 launch time, around 11:00 UTC, depending on the day. This time window is sufficient
 330 to average across individual cloud-turbulence elements yet brief enough to prevent al-
 331 terations in the overall large-scale atmospheric conditions.

332 The prognostic humidity budget equation in *DALES* is formulated in terms of $q_t =$
 333 $q_v + q_l$ as the total humidity and excludes suspended cloud ice which is treated as a sep-
 334 arate prognostic variable. To achieve an internally consistent initialization of all humid-

335 ity state variables, q_v , q_l , and q_i are combined in a height-dependent way, as follows. In
 336 areas of expected turbulent ice production (below z_{cut} , see equation (B7)), the ice and
 337 liquid water specific mixing ratio are added and given to the model as only liquid. The
 338 expected behavior of the model is to convert the additional liquid into ice via the mi-
 339 crophysics scheme and represent accurate IWC and LWC distributions after a spin-up
 340 phase. In areas of expected deposition ice production (above z_{cut}), the retrieved IWC
 341 is directly included in the model. If ice is measured, the model will place ice clouds di-
 342 rectly with an estimated effective radius of $55 \mu\text{m}$. This shortens the lengthy deposition
 343 spin-up process and produces realistic, weakly turbulent, high-level ice clouds.

344 The initial profile of the cloud condensation nuclei (CCN) concentration in the *DALES*
 345 mixed-phase microphysics scheme (see 2.2.2) are estimated based on the observations
 346 from the *Cloud Condensation Nuclei Particle Counter* located aboard *Polarstern* (Koontz
 347 et al., 2020). The measurements show high seasonal and day-to-day variability, as well
 348 as variability during some days. However, with an emphasis on the consistency of the
 349 setup, the mean value of each day is used as the initial value of CCN concentration for
 350 the simulation. The value from the preceding recorded day was used for days missing
 351 data. In the absence of a consistent CCN profiling of the Arctic air, the measurements
 352 in the bottom part of the atmosphere are considered a good proxy for the conditions in
 353 the rest of the boundary layer.

354 The number concentration of activated ice nucleating particles (INP) is not yet treated
 355 prognostically in the current version of the *DALES* microphysics scheme. In the code,
 356 the INP concentrations are determined from temperature-dependent activation spectra
 357 (Seifert & Beheng, 2006), prescribed by exponential functions with constant parameters
 358 proposed by Reisner et al. (1998). Laboratory measurements of INP activation from in-
 359 situ samples of Arctic air extracted near *Polarstern* during *MOSAiC* (Creamean et al.,
 360 2018; Creamean, 2022) showed a high time-variation in activation spectra, motivating
 361 initialization with daily observed values. The associated observed INP number concen-
 362 trations were significantly lower than the values proposed by the parameterization men-
 363 tioned above, often by more than two orders of magnitude. To keep the simulations as
 364 representative as possible of the observed atmosphere, the measured activation spectra
 365 were used instead. A logarithmic regression was applied to each measured spectra from
 366 the laboratory samples, and the resulting slope and intercept parameters were then in-
 367 serted as new values in the deposition-nucleation scheme instead of the original constant
 368 values. Finally, limitations in the sampling of the spectra during the drift necessitate adopt-
 369 ing two further simplifications in the initialization of the INP profile in the model. Firstly,
 370 due to the three-day sampling rate, the spectra on sampling-free days are set at the val-
 371 ues from the last preceding day of availability. Secondly, due to the absence of consis-
 372 tent and continuous INP profiling during the drift, the activation spectra are simply as-
 373 summed constant with height.

374 **2.3.3 Lower boundary conditions**

375 Similar to the initial profiles, the lower boundary conditions for model variables
 376 are mainly based on *MOSAiC* data. Additional information is taken from the ERA5 re-
 377 analysis. The boundary conditions are prescribed, constant in time, and horizontally ho-
 378 mogeneous in the simulated domain.

379 The sea-ice fraction at the location of the *Polarstern* is taken from ERA5 reanal-
 380 ysis data. With the research vessel frozen in solid pack ice for most of the simulated days,
 381 the sea-ice fraction at the ship was often close to 100 %. Accordingly, short-time reduc-
 382 tions in the sea-ice fraction, for example, due to lead events, are not considered in the
 383 control experiments for simplicity but could simply be added in future sensitivity exper-
 384 iments.

As described in section 2.2.4, two surface skin temperatures are considered in the
DALES bulk surface parameterization; one for sea ice and one for open water. For the
 ice surface skin temperature T_{seaice} the brightness temperature measurements at the *MetC-*

ity installation are used (Cox et al., 2023). For the skin temperature of open water, the ocean temperature is used, which is assumed to follow

$$T_{\text{ocean}} = \max(T_{\text{seaice}}, -1.8^\circ\text{C}), \quad (2)$$

385 where the numeric value represents the typical freezing temperature of ocean water. In
 386 practice, and for consistency with the profile initialization described above, for T_{seaice}
 387 the surface value of the combined data product by Dahlke et al. (2023) is used. This value
 388 is the skin temperature measured at *MetCity*. Preliminary experiments demonstrated
 389 that the skin temperature is a crucial boundary condition to get right, as it directly de-
 390 termines the upward longwave radiation and strongly affects the low-level stability in the
 391 simulations. For this reason, no simulations were carried out for days on which *MetC-*
 392 *ity* data were not available. Using *ERA5* values as a replacement was no option for these
 393 days because i) this would introduce inconsistencies in the boundary conditions during
 394 the drift, and ii) warm biases are known to exist in the reanalysis regarding the surface
 395 skin temperature (Day et al., 2020). As a guiding principle, integrating different data
 396 sets in the simulation for the same quantity goes against the approach of a standardized
 397 setup.

398 **2.3.4 Surface properties**

399 The surface roughness length for momentum $z_{0,m}$ plays a key role in the Monin-
 400 Obukhov theory for calculating turbulent fluxes. Accordingly, adopting realistic values
 401 is important to get the flux boundary condition right. However, in many model appli-
 402 cations, including LES research, the surface roughness length is simply estimated, e.g.,
 403 ECMWF (2021); Michaelis et al. (2020). Fortunately, $z_{0,m}$ can be derived from daily *MO-*
 404 *SAiC* data of the near-surface wind, turbulence, and temperature measurements (Cox
 405 et al., 2023; Gallagher, 2023). This data provides an accurate boundary condition for
 406 $z_{0,m}$ for each simulated day. In the literature the surface roughness length for heat $z_{0,h}$
 407 in the Arctic is often assumed as $z_{0,h} = 0.1 \cdot z_{0,m}$ (e.g. IFS Model ECMWF (2021);
 408 Michaelis et al. (2020)). For lack of direct measurements of $z_{0,h}$ during the drift, this value
 409 is also adopted here for the control experiments.

410 The final boundary condition to be considered concerns the surface albedo α . Dur-
 411 ing polar day, the reflectivity of the predominantly frozen surface directly controls the
 412 solar contribution to the surface energy budget. The horizontal scale that α represents
 413 is set by the horizontal dimension of the simulated domain. Landscape features such as
 414 melt ponds and leads are known to affect the average reflectivity of an area on a meter
 415 to kilometer scale (Niehaus et al., 2023), while Arctic weather also influences surface prop-
 416 erties on much larger scales. To capture both effects at once, the satellite α product de-
 417 scribed by Spreen et al. (2008); Istomina et al. (2020) is adopted here. Two main issues
 418 affect the accuracy of the satellite estimates of surface albedo; cloud cover and limited
 419 satellite overpasses. As a result, satellite albedo products often have significant spatial
 420 and temporal gaps. To address this, a rolling average over a week-long period is used to
 421 smooth out as many inconsistencies as possible in the data. Secondly, spatial interpola-
 422 tion in the resulting maps gives a reasonable estimate of the albedo in areas around
 423 *Polarstern*. It is possible, that the interpolation in time and space introduces an albedo
 424 bias toward cloud-free conditions. A further improvement was not considered for two rea-
 425 sons. Albedo measurements for cloudy conditions would be derived from a second dataset,
 426 which clashes with the standardized setup. Secondly, the uncertainty by this bias is ex-
 427 pected to be small when used in the simplified radiation scheme employed in *DALES*.

428 **2.3.5 Large-scale forcing and nudging**

429 The simulated portion of the atmosphere is not isolated from the larger-scale flow
 430 in which it is embedded. Various larger-scale processes impact the development of the
 431 atmospheric boundary layer, including large-scale advection, vertical motion, and pres-
 432 sure gradients. In *DALES*, these forcings are considered and applied in a horizontally

433 uniform way, while maintaining height-dependency. The associated tendencies are either
 434 fully prescribed or partially interactive with the domain-average profile. This forcing method
 435 is described in detail by van Laar et al. (2019) and is, in principle, adopted here, with
 436 a few notable exceptions as described below.

In the prognostic budget equations for $\varphi \in \{q_t, \theta_1, u, v\}$ the tendency due to large-scale subsidence S_φ^{subs} is constructed using a prescribed large scale vertical motion w_s and the local vertical gradient, calculated from the vertical profile of the domain averaged variable $\bar{\varphi}$,

$$S_\varphi^{\text{subs}} = -w_s \frac{\partial \bar{\varphi}}{\partial z} \quad (3)$$

(Siebesma et al., 2003). This means the significant impact of subsidence on inversions is captured. In the momentum equations the pressure gradient (p) and Coriolis (f) forces are represented in combination, through the departure of the actual wind from the geostrophic wind,

$$S_u^{\text{p+f}} = -f(\bar{v} - \bar{v}_g), \quad (4)$$

$$S_v^{\text{p+f}} = f(\bar{u} - \bar{u}_g), \quad (5)$$

437 with f the latitude-dependent Coriolis parameter and subscript g indicating the geostrophic
 438 state. The latter is calculated from the horizontal pressure fields from ERA5.

439 In the standardized case generation, the time and location of the *Polarstern* at 11:00
 440 UTC are determined first. Then the six-hour upstream trajectory of the 950 hPa air mass
 441 is estimated from the ERA5 reanalysis data. The quantities required for calculating the
 442 forcing terms are then calculated at all trajectory points across an area of 1×1 degrees,
 443 using the Lagrangian perspective described by Neggers, Chylik, et al. (2019). This means
 444 all horizontal advective terms are zero per definition at the height of diagnosis (950 hPa).
 445 Finally, the forcing terms are then time-averaged over six hours preceding the arrival of
 446 the low-level air mass at the *Polarstern*. This yields time-constant composite forcings,
 447 which express how the air mass was modulated by larger-scale processes during the pe-
 448 riod in which any clouds observed at the *Polarstern* formed. To limit the influence of large-
 449 scale processes on the evolution of the simulated domain, horizontal advection of tem-
 450 perature and moisture is set to zero. This approach isolates boundary layer processes
 451 as drivers of atmospheric changes.

Continuous Newtonian nudging is applied above the boundary layer thermal inversion to prevent excessive drift of the upper part of the troposphere (Randall & Cripe, 1999; Sobel & Bretherton, 2000; Derbyshire et al., 2004; Neggers et al., 2012). The nudging tendency S_φ^n is formulated in terms of the spatially averaged profiles (Heus et al., 2010; Neggers et al., 2012),

$$S_\varphi^n = -\frac{1}{t^n} (\bar{\varphi} - \varphi^n). \quad (6)$$

Here, $\bar{\varphi}$ is the horizontal mean of an arbitrary scalar, t^n is the nudging time scale, and φ^n is the profile towards which the model profile is relaxed, which in this case is the initial profile based on the corrected 11:00 UTC radiosonde data. The nudging time scale is set to $t^n = 10\,800$ s. It is only applied above the boundary layer height z_i , which is adaptively calculated based on the maximum liquid water potential temperature gradient. This method is well established in the literature, e.g., (Sandu & Stevens, 2011; Zhang et al., 2013; Neggers et al., 2017). Height z_i as used to define the bottom of the nudging layer is defined to be situated in a specified range, as follows:

$$z_i, \text{ where } \left. \frac{\partial \Theta_v}{\partial z} \right|_{z=z_i} = \max \left(\left. \frac{\partial \Theta_v}{\partial z} \right|_z \right), z \in [100 \text{ m}, 5000 \text{ m}] \quad (7)$$

452 This specification is a practical protection against artificially high gradients near the sur-
 453 face and the tropopause inversion.

454 The final external forcing to be discussed is the radiative forcing at the top of the
 455 simulated domain. The downward radiative fluxes at the model ceiling are calculated
 456 by including the part of the full radiosonde (initial) profile in the radiative flux calcu-
 457 lations that is situated above the ceiling. This way, impacts of the upper atmosphere on
 458 both longwave and shortwave radiative transfer are represented as a soft and interactive
 459 boundary condition.

460 3 Results

461 With the initialization, boundary conditions, and large-scale forcing thus defined,
 462 an experimental configuration is obtained with the following key characteristics;

- 463 • The simulated domain represents a statistical, homogeneously forced downscal-
 464 ing of the mean atmospheric column as observed daily at 11:00 UTC at the *Po-*
 465 *larstern* during *MOSAiC*;
- 466 • The recent history of the low-level air mass is represented through Lagrangian forc-
 467 ing;
- 468 • Time-composite forcing means the simulations can quasi-equilibrate, depending
 469 on the proximity to a balance in the prognostic budget equations;
- 470 • Resolved, small-scale boundary layer processes are free to evolve below the ther-
 471 mal inversion;
- 472 • Mixed phase clouds are allowed to spin up and interact with radiation, resolved
 473 dynamics, and prognostic aerosol.

474 This model configuration was arrived at after extensive testing on both smaller and larger
 475 grids. A three-dimensional volume rendering of a mixed-phase cloud that results from
 476 this setup is shown in figure 1 to illustrate that the turbulent dynamics in which these
 477 clouds are embedded are resolved to a high degree with this setup. The presentation of
 478 the results with this model setup is subdivided into three parts. Section 3.1 provides an
 479 overview of the successfully simulated cases during the year-long *MOSAiC* drift. Sec-
 480 tion 3.2 presents the statistical evaluation of the model output against a year of *MO-*
 481 *SAiC* data, and includes a brief initial discussion on data comparability. Section 3.3 fo-
 482 cuses in more detail on three selected days, to gain insight into the typical behavior of
 483 single simulations and to explore the potential use of the generated library of simulations
 484 for further scientific research.

485 3.1 Simulation overview

486 Figure 2 gives an overview of the days during the *MOSAiC* drift that were success-
 487 fully simulated in the PRODUCTION setup featuring the highest resolution and the largest
 488 domain, as described in Table 2. Here, success implies two things:

- 489 • The data needed for the standardized setup is complete and available at 11:00 UTC;
- 490 • No numerical issues occurred, and the simulation was completed successfully.

491 A subset of non-simulated days can be distinguished that is more or less randomly dis-
 492 tributed in time. On these days, typically, an observational dataset is missing that is part
 493 of the experimental setup. Two longer, continuous periods also exist that are not simu-
 494 lated; one in May-June 2020 and another in July-August. These coincide with the *Po-*
 495 *larstern* not being at the ice floe or *MetCity* not being operational. If not stated oth-
 496 erwise, all results discussed below represent the PRODUCTION setup.

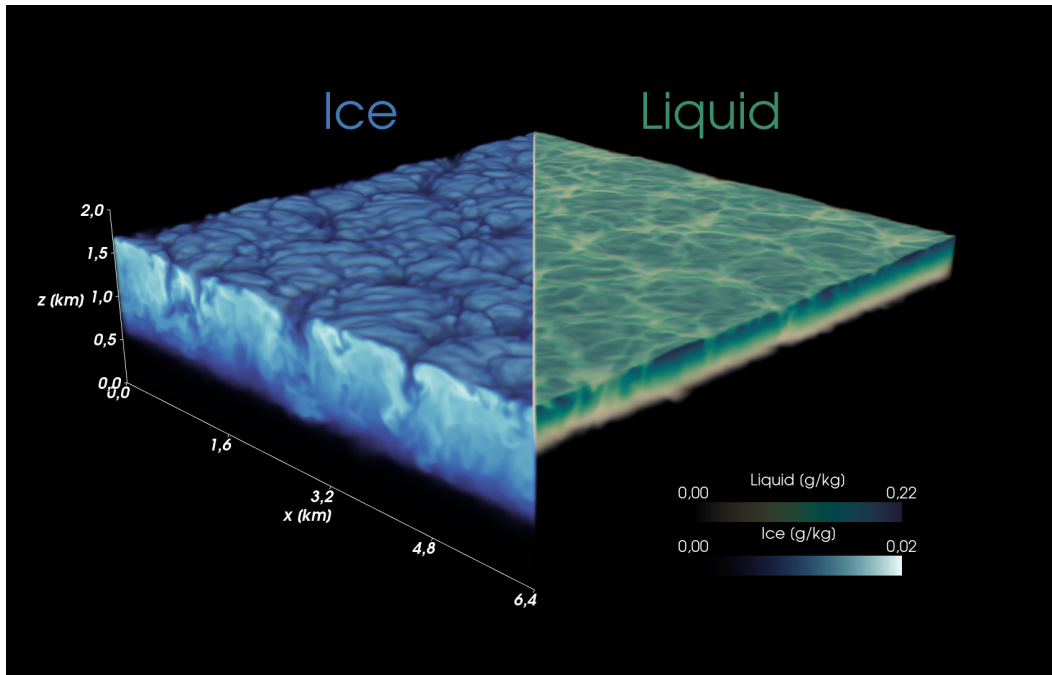


Figure 1. Volume rendering of the 20191101 case (see table 3) after 1.5 h of the full horizontal domain. The two quantities shown are the specific mixing ratios for ice (blue) and liquid (green) water. For visual reasons, the ice is only shown on the left, and the liquid only on the right.

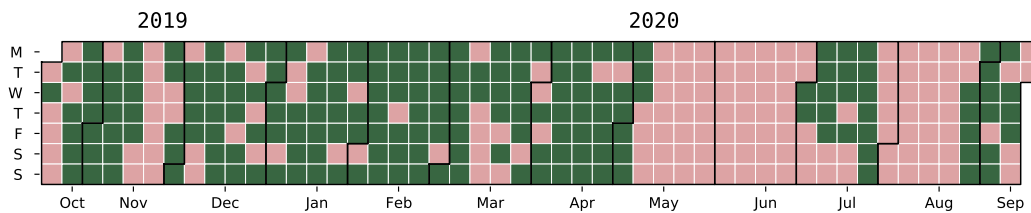


Figure 2. Overview of simulated case studies by date. Green indicates a successful simulation of the state of the boundary around 11:00 UTC at the *Polarstern*. Red shows days on which simulations were unsuccessful.

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3.2 Statistical evaluation

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The objective of this section is to evaluate the library of daily LES experiments against the year-long record of *MOSAIC* data. The general approach is to assess the difference between simulated values and their measured counterparts for selected variables to identify both strengths and weaknesses of the library of simulations concerning resolved aspects of the Arctic boundary layer and the surface energy budget. When interpreting the simulations and comparing them to measurements, three important considerations should be made, as briefly discussed here.

The first consideration is the *state of equilibrium* of the simulated and observed boundary layer. When the sum of all sources and sinks in the bulk ABL budget is non-zero, a net tendency exists that can gradually warm, cool, moisten, or dry the layer. Due to our lack of knowledge of these tendencies in nature, it remains unknown if the observed ABL is close to equilibrium or not. The simulated ABL can similarly be out of equilib-

rium, for example, through uncertainties in the applied forcings. However, what helps in model-observation comparability is the well-known slow adjustment of Arctic boundary layers, reflecting that net bulk tendencies are small compared to individual budget terms (Neggers, Chylik, et al., 2019). Another convenient factor is the observed persistence of ABL-related phenomena such as clouds (Shupe et al., 2006; Shupe, 2011; Stramler et al., 2011; Morrison et al., 2012), which implies that the model budget should be pretty similar to the observed one when initializing with observed cloud profiles. For these reasons, it is assumed a priori that the simulated ABL is, in principle, comparable to its observed equivalent. When doing so, one still needs to determine the optimal time point after initialization at which a comparison can be made. On the one hand, turbulent-cloudy processes need to spin up properly; on the other, significant drift from the desired state can happen and needs to be minimized. Careful equilibration analysis of all simulations yielded an optimal time point of 1.5 h after initialization. More details about this analysis can be found in Appendix C.

The second important consideration in the evaluation effort is the *independence of the observational data* from the numerical experiments. What is relevant is that the latter are already closely based on *MOSAIC* datasets. Ideally, one should evaluate resolved processes in the LES against completely independent datasets. This is indeed the case for a large subset of evaluation datasets, such as the surface radiative and turbulent energy fluxes. However, in principle, cloud properties are far less independent from the simulations, as these are initialized with observed cloud profiles. Nonetheless, it should be noted that clouds in the model can significantly evolve during the simulated period before the sampling time point due to strong interactions between thermodynamics, turbulence, and radiation. Accordingly, it is far from trivial that clouds remain unchanged from their initial state. This makes comparison to the observed cloud properties meaningful; a close agreement reflects model skill in maintaining the turbulent cloud layer.

The third consideration is about *uncertainties* in the observational datasets and how to deal with them in the model evaluation. A complicating factor is that these uncertainties also flow into the model setup through the initialization and boundary conditions. How these errors percolate into the final simulation, and to what degree, is hard to disentangle and even harder to isolate from other error sources such as numerics and the prescribed forcings. For these reasons, it was decided to exclude error bars in the evaluation plots. A thorough error analysis is for now considered future work.

3.2.1 Radiative energy fluxes

3.2.1.1 Longwave radiation Figure 3 shows scatter plots of the simulated versus observed near-surface longwave radiative fluxes at the *MetCity* site located on the ice floe near the *Polarstern* (Cox et al., 2023; Riihimaki, 2021). Included are the a) upward, b) downward, and c) net fluxes at 1–3 m height. The simulated upward flux reproduces the observed values to a high degree, in part because the surface skin temperature used in the simulations is derived from these radiation measurements. The good agreement confirms that the radiation scheme accurately represents the radiative energy emitted by the surface. A slight warm bias exists, which is introduced by the use of the double skin temperature as described in Section 2.3.3. The radiation scheme also uses this combined skin temperature (weighted by the sea-ice fraction) as the surface emission temperature for the wider area, while the measured fluxes purely reflect the local temperature of the (colder) sea ice on which they were made.

For the longwave downward flux (that indirectly reflects cloud presence) the agreement is also satisfactory, especially for the upper and lower tails of the distribution (Fig. 3b). This agreement indicates that the model does a reasonable job of simulating both the atmospheric temperature and the vertical location and presence of clouds. In the lower intermediate range, some positive outliers exist. To gain insight, Fig. 4 shows the same data but now shaded according to the (a) ice water path (IWP) and the (b) liquid water path (LWP). This additional information reveals that good agreement exists for i)

563 cold and cloud-free conditions ($LW_{\text{down}} \leq 120 \text{ W m}^{-2}$) as well as ii) warm and opti-
 564 cally thick liquid clouds ($LW_{\text{down}} \geq 200 \text{ W m}^{-2}$). The intermediate range suffers from
 565 a well-defined bias for relatively high IWP values, suggesting too high emissivity by thick
 566 ice clouds in the model. A deeper investigation of high-bias days revealed that the er-
 567 ror is introduced by parametric assumptions in the *DALES* radiation scheme concern-
 568 ing the effective diameter of ice crystals. An effective diameter range of 20–120 μm is
 569 applied, which was originally developed for cirrus clouds. Ice crystals in the Arctic can
 570 be observed to exceed that value (Shupe et al., 2006). Capping ice diameters at a too-
 571 small value leads to the overestimation of the optical thickness of ice clouds. Addition-
 572 ally, it is uncertain if the mean particle radius calculated by the bulk microphysics scheme
 573 can be used with proportional ratio 1 as the radiative effective radius in the radiation
 574 scheme. These sensitivities are discussed further in section 4.

575 Combining the upward and downward fluxes yields the net flux (Fig. 3c). The data
 576 shows the bimodal distribution typical of the Arctic, which is reproduced to a reason-
 577 able degree by the simulations and is explored in more detail in Section 3.2.4. While a
 578 general agreement exists with the observations, as expressed by the relatively low bias
 579 compared to the mean signal, the error introduced by the biases in the longwave down-
 580 ward radiation for ice clouds now materializes much more pronouncedly. Analysis indi-
 581 cates that the model particularly struggles in situations with optically thin ice clouds,
 582 claiming unrealistically low magnitude net radiative fluxes close to 0 W m^{-2} .

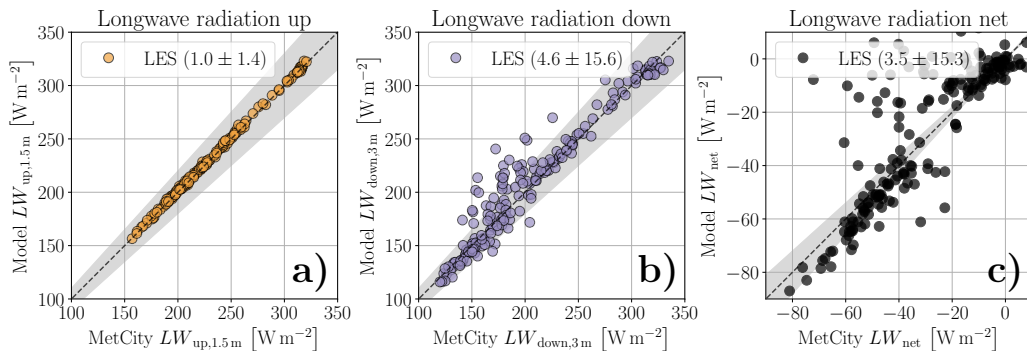


Figure 3. Scatter plots of simulated versus observed a) upward, b) downward, and c) net longwave radiative fluxes. LES results (ordinate) are plotted against *MetCity* tower measurements (abscissa). Each dot represents a single simulated daily case. The simulation is sampled at $t = 1.5 \text{ h}$ after initialization, while the measurement represents the 15 min average after radiosonde launch time. The dashed line indicates the one-to-one diagonal. The gray shading indicates the $\leq 10\%$ difference area, for reference. Values in the legend show $\mu \pm \sigma$, with μ and σ being the mean and standard deviation of simulated minus measured values, respectively.

583 **3.2.1.2 Shortwave radiation** Figure 5 compares the simulated and observed near-
 584 surface shortwave radiative fluxes. Non-zero values indicate polar spring and summer
 585 and reflect model performance during the melt season. When interpreting these results,
 586 it is important to realize that *DALES* only considers purely vertical radiative transfer.
 587 This assumption is commonly made in most atmospheric models, including most present-
 588 day LES codes, with only a few notable exemptions. However, it is also a significant sim-
 589 plification of reality that excludes three-dimensional radiative effects, which might in-
 590 troduce biases for low solar zenith angles, as are typical of the Arctic during polar day.
 591 With this in mind, the model biases in shortwave fluxes are largest at small values and
 592 decrease significantly as the shortwave fluxes increase. In terms of energy flux units, the

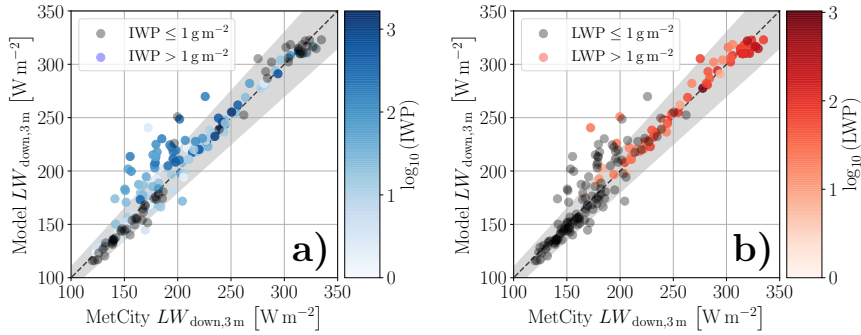


Figure 4. Similar to Fig. 3 b, but now shown with data points color-coded based on the simulated a) ice water path (IWP) and b) liquid water path (LWP).

593 bias and spread are somewhat larger compared to the longwave fluxes. For all three fluxes,
 594 the bias is negative, suggesting that too little shortwave energy is entering the system.
 595 This might be due to the exclusion of three-dimensional effects, a hypothesis that needs
 596 testing in future research. One notices that the distribution of data points in the upward
 597 and downward flux figures is structurally similar. In combination with the accuracy of
 598 the upward flux and in association with the resulting net flux, one concludes that the
 599 prescribed albedo boundary condition must be close to the true value. This skill was only
 600 arrived at after including the satellite-based albedo measurements (not shown).

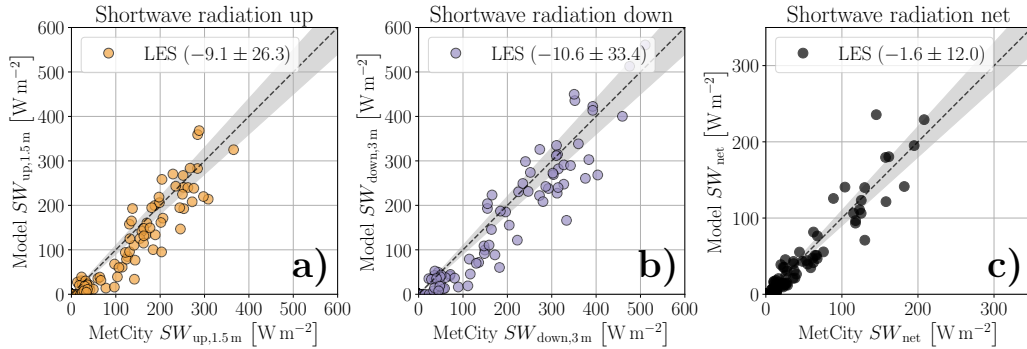


Figure 5. Similar to Fig. 3 but now showing the a) upward, b) downward, and c) net short-wave radiative flux at the surface.

3.2.2 Water paths

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602 Two well-known and critical success metrics for reproducing clouds in the virtual
 603 domain are the liquid water path (LWP) and the ice water path (IWP). Figure 6 shows
 604 the comparison of simulated and measurement-based values for (a) IWP and (b) LWP.
 605 Focusing first on the ice, the general trend of measured IWP is well reproduced by the
 606 model. Measurements and model data agree for most cases. Nonetheless, several sim-
 607 ulations under- or overestimate the amount of ice in the column. When interpreting these
 608 outliers it should be taken into account that the simulations are initialized with the ob-
 609 served profiles of liquid and ice cloud water. Accordingly, in these cases, the offsets arise
 610 during the simulated period, which points at the model experiencing difficulties main-

611 taining the right ice amount. Possible causes for this trend include i) lack of resolution
 612 to fully resolve cloud-forming dynamical processes in the upper atmosphere, ii) uncer-
 613 tainties in the applied large-scale forcings, and iii) lack of skill in the microphysics scheme.
 614 At this point, it is not clear which of these causes apply. However, encouraging aspects
 615 are that the model always maintains at least some ice and that the outliers seem ran-
 616 domly scattered around the correct mean as calculated over the full drift.

617 The measured LWP is mostly well captured by the simulations. A few cases un-
 618 derestimate the amount of liquid. This underestimate can happen when freezing rates
 619 are overestimated by the model and liquid clouds glaciate too eagerly. The most signif-
 620 icant relative errors for LWP and IWP occur in the region $\leq 50 \text{ g m}^{-2}$. Closer inspec-
 621 tion of these cases suggested that in situations with really thin ice and liquid clouds, the
 622 model is increasingly sensitive to the initial conditions. On the positive side, it can be
 623 considered a success that the model can capture and reproduce these thin clouds in the
 first place, to some degree.

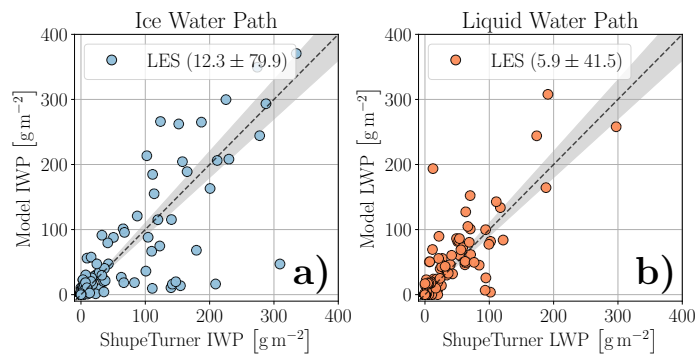


Figure 6. Scatter plot of simulated versus observed a) Liquid Water Path (LWP) and b) Ice Water Path (IWP). The LES is plotted against the ShupeTurner data set. Sampling, notation, and plotting style are analogous to the previous figures.

624

625 3.2.3 Near-surface meteorology

626 Figure 7 shows the simulated versus observed (a) wind speed, (b) temperature, and
 627 (c) sensible heat flux at 10 m height. The wind speed in the simulation compares well
 628 to the measurements, which is especially gratifying since the wind profile given to each
 629 simulation as initial condition stems from *ERA5* reanalysis data. The *MOSAiC* radiosonde
 630 data were assimilated into *ERA5*. Simulation forcings and near-surface turbulence can
 631 cause differences from the initial profile after the spin-up phase. For these reasons, a good
 632 agreement is not trivial. Nonetheless, the relative error can be high for low wind speeds,
 633 and the impact on near-surface transport processes is significant. The simulation is bi-
 634 ased towards lower values for wind speeds $\geq 10 \text{ m s}^{-1}$. Low-level jets are a common phe-
 635 nomenon in the high Arctic (López-García et al., 2022), and their underestimation in
 636 the LES might explain this small bias.

637 Figure 7 b shows that the simulated 10 m temperatures closely resemble the ob-
 638 servations. This is arguably not surprising, given i) the prescribed observed skin tem-
 639 perature as measured at *MetCity* and ii) the radiosonde temperature profile being part
 640 of the model initialization. The close agreement at least confirms that the simulation has
 641 not drifted away from the measured thermodynamic state after the spin-up period.

642 Figure 7 c evaluates the simulated 10 m sensible heat flux (H_s). By convention, a
 643 positive sign indicates an upward flux. In general, the observed distribution and orien-

644 tation of the data points in this space are reproduced, but the mean bias and spread are
 645 relatively large compared to the mean signal. The mean bias is negative, expressing a
 646 general underestimation of the flux of sensible heat between surface and atmosphere. Sig-
 647 nificant negative biases occur on individual days, which are responsible for most of the
 648 mean bias and spread. On some days, the underestimation reaches more than 20 W m^{-2} .

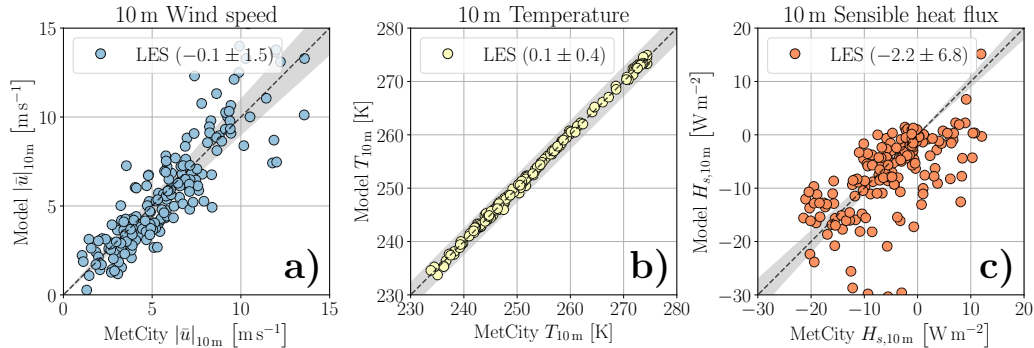


Figure 7. Scatter plots of simulated versus observed meteorological properties at 10 m height, including (a) wind speed, (b) temperature, and (c) bulk sensible heat flux. Sampling, notation, and plotting style are analogous to the previous figures.

649 The surface H_s is a key player in the SEB, an important aspect of the Arctic cli-
 650 mate system, which is crucial to correctly represent in model realizations. Accordingly,
 651 it is imperative to gain an understanding of these large differences between the model
 652 and measurements. Before claiming model shortcomings, it is relevant to first consider
 653 data comparability. At least both the model and observed fluxes rely on bulk methods.
 654 The observed fluxes were calculated using the method developed by Fairall et al. (1996),
 655 making use of turbulent transfer coefficients and roughness length estimated from the
 656 *Surface Heat Budget of the Arctic Ocean (SHEBA)* campaign (Andreas et al., 2003). For
 657 a more detailed description refer to Cox et al. (2023). As described in Section 2.2.4, the
 658 simulations also make use of stability functions based on SHEBA data (Grachev et al.,
 659 2007). But the use of roughness lengths based on daily *MOSAiC* measurements in the
 660 simulations is a key difference. Adopting the transfer coefficients and roughness lengths
 661 improved the simulations from the first attempts in terms of the H_s (not shown). How-
 662 ever, potential differences with the SHEBA roughness lengths could explain some of the
 663 remaining outlying data points.

664 More causes can be thought of to explain the differences in the H_s . These include
 665 i) local impacts on the measured fluxes not accounted for in the simulations and ii) the
 666 possible inapplicability of Monin-Obukhov similarity theory over sea ice in stable winter-
 667 tertime conditions (Heisel & Chamecki, 2023). An interesting alternative data source for
 668 comparison with the LES could be the eddy-covariance flux product that is part of the
 669 *MOSAiC* data archive (Cox et al., 2023). Further investigating these research questions
 670 is for now considered future work. The library of LES experiments presented in this study
 671 can inform this effort by providing situations for which large differences occur.

672 3.2.4 The bimodal Arctic

673 The surface energy budget of the Arctic is dominated by two primary modes. The
 674 first reflects cold, clear, and stable conditions, while the second represents warmer, cloudy
 675 states with often neutral or weakly unstable near-surface conditions. This bimodal na-
 676 ture of the Arctic climate system is a long-known phenomenon (Sverdrup, 1933) and has
 677 been measured extensively during previous drift campaigns like SHEBA (Persson et al.,

1999, 2002; Shupe & Intrieri, 2004; Stramler et al., 2011). The bimodal state has been intensely researched in recent years, given its importance in Arctic Amplification and sea ice melt. In particular, transitions between the dominant modes have been a topic of interest. Previous modeling efforts have contributed to our insight, for example, by linking the bimodality to mixed-phase cloud persistence (Morrison et al., 2012) and large-scale dynamics (Neggers, Chylík, et al., 2019). Also, well-defined bimodality has been used as a metric to test the skill of climate and single-column models (Pithan et al., 2014, 2016; Solomon et al., 2023). Because small-scale dynamics are resolved in LES instead of being parameterized, one expects a priori that the library of *MOSAIC* simulations, as discussed here, should have some skill in reproducing this feature. The availability of 190 realizations under a broad range of atmospheric conditions should provide a sufficient sample size to reproduce the bimodal distribution. These questions are addressed in this section .

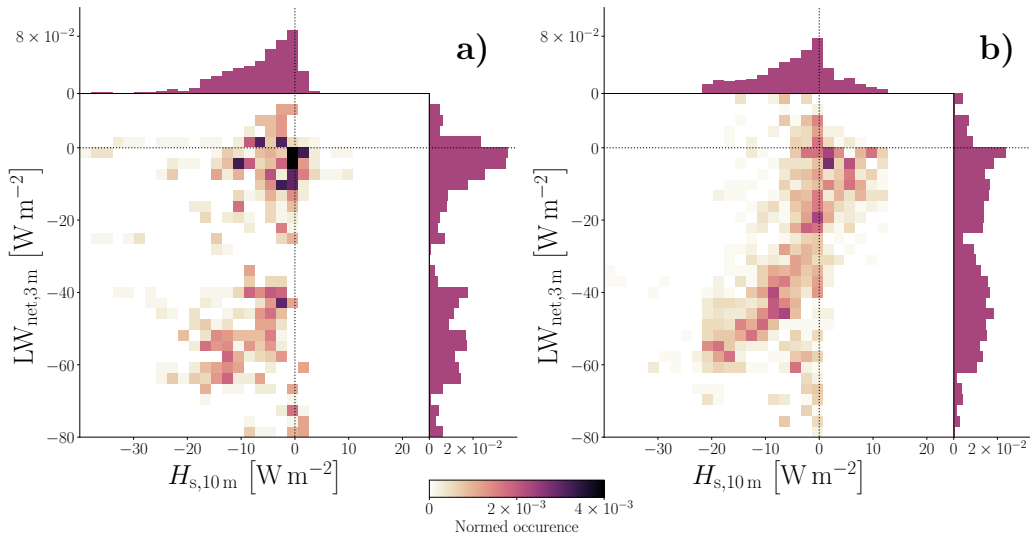


Figure 8. Two-dimensional histograms of normalized occurrence of atmospheric states characterized by the near-surface net longwave radiation (ordinate) and sensible heat flux at 10 m height (abscissa). (a) shows the LES results in which each data point of the given quantities is averaged over 15 min and the whole domain from every simulated case. (b) shows the measured values from *MetCity* (Cox et al. (2023); Fairall et al. (1996), "*bulk-Hs_10m*") between 10:45 UTC and 11:15 UTC daily.

Figure 8 shows the two-dimensional probability density function (PDF) of near-surface longwave net radiation (LW_{net}) and the near-surface sensible heat flux (H_s), as a) sampled from the year-long library of LES experiments and b) as observed during *MOSAIC*. These two variables were previously discussed individually in Sections 3.2.3 and 3.2.1, respectively, but are combined here. The bimodality is visible in the measurements, with the modes best defined along the LW_{net} axis. A variety of states is observed between the cloudy mode (near the origin) and the clear mode (bottom left). For convenience, the PDFs are also shown separately as side panels, to better determine and compare the mode locations.

For comparing the model to the measurements the two modes are now considered individually. The cloud-free mode ($LW_{\text{net}} \leq -30 \text{ W m}^{-2}$) is nearly always accompanied by a negative H_s , which can be as low as -30 W m^{-2} for extremely cold surface conditions. The model correctly reproduces this mode, although the diagonally-shaped maximum is shifted somewhat towards more negative LW_{net} values. The particularly inter-

esting cluster of cases with extremely low LW_{net} but near-zero H_s is also well captured by the model. The cloudy state ($LW_{\text{net}} > -30 \text{ W m}^{-2}$) in the LES is situated near the observed one, with a maximum occurrence of LW_{net} around 0 W m^{-2} . However, the LES fails to capture the observed weakly positive H_s occurrences and in general, is biased towards lower heat flux values (as discussed previously in Section 3.2.3). Part of a possible explanation for this underestimation could be the absence of leads in the simulations, which are known to locally boost the sensible and latent heat flux (Li et al., 2020). Additional sensitivity experiments at this location of the phase space could be informative, especially because Cox et al. (2023) note that they are likely to also miss lead effects in their bulk heat flux calculations.

A closer comparison of the simulated and observed LW_{net} side panels suggests that the LES slightly underestimates the number of intermediate states between the two dominant modes. This is also visible in the two-dimensional phase space. What causes the absence of these intermediate states in the LES is not yet fully understood, and is currently under investigation. Part of the issue could be related to the misrepresentation of longwave radiation emitted by ice clouds discussed in section 3.2.1. More possible causes include the absence of mesoscale variability in the numerical realizations due to spatially homogeneous forcing and small domain size, or an underestimation of cloud-transitional states due to characteristics of the experimental setup.

3.3 Case studies

The statistical evaluation against the full year of data in section 3.2 provides confidence in the basic skill of the LES in reproducing the cloud-radiative climate and surface energy budget of the central Arctic. This section explores a subset of three simulations in more detail. Each simulation serves as a case study of a different Arctic boundary layer, selected to accentuate results of particular interest. Table 3 gives an overview of these cases. The goal is to document resolved boundary-layer processes such as turbulence, and associated features such as vertical structure, inversions, and mixed-phase clouds. This is motivated by the potential use of these virtually resolved data sets in future research efforts.

3.3.1 Vertical structure

Figure 9 shows the potential temperature Θ , the ice q_i , liquid q_l and vapor q_v specific humidity profiles for the three cases. Analogous to previous sections, the simulations are evaluated after 1.5 h run time. The observational data sets served as initial conditions for the simulations. The value of comparing the simulation to its initial conditions is to judge how well the numerical experiment can keep the measured atmosphere in the virtual domain after the spin-up phase.

Table 3. Overview of exemplary case studies shown in section 3.3

Name	Date	Description
20191101	01 November 2019	Single layer mixed-phase cloud
20200216	16 February 2020	Mixed-phase cloud with thin ice cloud above
20200310	10 March 2020	Extremely cold icy atmosphere

The first case simulates the atmosphere measured around the *Polarstern* on November 1, 2019 at 11:00 UTC. Figure 9a-c gives an overview of the results. The boundary layer contains a well-mixed layer decoupled from the surface, as seen from the potential temperature in panel (a). The temperature inversion at 1750 m caps a mixed-phase cloud

745 seen in panel (b). It contains significant mass of liquid at the height 1200–1750 m and
 746 a minimal amount of ice at 600–1750 m. Here, the mixed-phase cloud is maintained,
 747 and the measured liquid and ice water content is reproduced. Only the ice layer around
 748 250 m measured by the ShupeTurner data sets is not found in the simulation. While tur-
 749 bulent processes intensify, the temperature and humidity profile remain nearly unchanged.
 750 Only a slight elevation and cooling of the temperature inversion is observed, as expected
 751 for a typical Arctic mixed-phase cloud.

752 The simulation for February 16, 2020 at 11:00 UTC shares several characteristics
 753 with the *20191101* case. As seen in figure 9d-f, a decoupled mixed-phase cloud is mea-
 754 sured at the *Polarstern* and reproduced by the LES. Additionally, in the spin-up time
 755 between the measurement and the evaluation of the simulation, the temperature inver-
 756 sion has lifted slightly while the cloud layer has cooled and water vapor has been depleted.
 757 In contrast to the first case, the cloud sits closer to the surface and is topped with a hu-
 758 midity inversion layer around 700 m. A clear success is the ability to maintain this hu-
 759 midity inversion right above the cloud top. The right balance between the entrainment
 760 of air above into the cloud layer and cloud-top cooling is crucial in simulating the longevity
 761 of mixed-phase clouds. The simulated liquid water profile has a maximum slightly be-
 762 low the cloud top, which is likely a more accurate profile shape than the simple adiabatic
 763 profile shape assumed in the observation-based estimate.

764 The final case discussed simulates March 10, 2020 at 11:00 UTC. It is character-
 765 ized by an extremely low boundary layer temperature, as can be seen in figure 9g. Fur-
 766 ther, panel (h) shows a significant amount of ice, especially considering the low amount
 767 of total moisture contained in the lower atmosphere (panel (i)). The large amount of ice
 768 well-distributed over the column is a typical situation for the Arctic. As discussed in sec-
 769 tion 2.3.2, ice, that is not expected to be produced by processes in turbulent clouds, is
 770 placed in the virtual domain as part of initialization. Despite the assumptions made, this
 771 simulation maintains an adequate amount of ice in the atmosphere while also depleting
 772 some of the water vapor during the 1.5 h run time. Additional research is needed to eval-
 773 uate if the model can reproduce accurate freezing rates and precipitation, as these are
 774 the main local source and sink processes for ice under extremely cold conditions.

775 **3.3.2 Mixed-phase cloud**

776 In Figure 10 the *20191101* case is shown in more detail. Panel a-c show the same
 777 vertical cross-section for the vertical velocity w , and the liquid and ice water specific hu-
 778 midities q_l and q_i . This is only one of dozens of single-layer mixed-phase clouds simu-
 779 lated in the collection of cases. In comparison to the previous discussion on the averaged
 780 vertical profiles, this figure shows the model’s capabilities in resolving the smaller-scale
 781 dynamics of mixed-phase clouds. The vertical velocity shows the up- and downdrafts in
 782 the cloud. Note, that here the downdrafts are stronger in magnitude than the updrafts,
 783 since cloud turbulence is mainly driven by cloud-top cooling. This skewness of the ver-
 784 tical velocity distribution is documented in past measurements (Shupe et al., 2013). As
 785 seen before, the typical vertical distribution of ice and liquid in mixed-phase clouds is
 786 shown: A relatively shallow liquid cloud is the source region for the formation of ice crys-
 787 tals that fall below the liquid cloud base. In this plot, the heterogeneity in the horizon-
 788 tal directions can be observed. There is a visible positive correlation between the ver-
 789 tical velocity and the liquid and ice water. Updrafts supply plentiful moisture to form
 790 and grow both cloud liquid and ice, while downdrafts entrain unsaturated air from above
 791 into the cloud. A detailed investigation of the interaction between turbulent, thermo-
 792 dynamic, radiative, and microphysical processes in Arctic mixed-phase clouds will be a
 793 future topic of research.

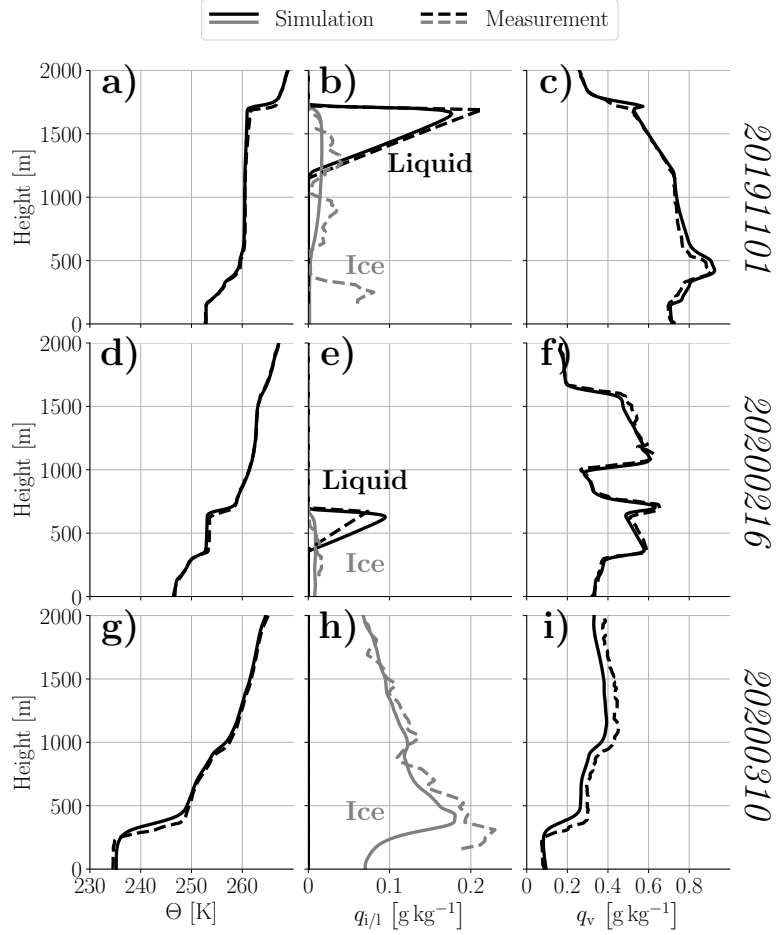


Figure 9. Analysis of the vertical profiles of potential temperature Θ , ice and water specific mixing-ratio $q_{i/l}$, and water vapor specific mixing-ratio q_v for the cases *20191101* (a-c), *20200216* (d-f) and *20200310* (g-i). Shown are the simulation results averaged over 15 min in time and over the whole domain in space after 1.5 h run time (solid) and observations at radiosonde launch time around 11:00 UTC (dashed). Observed Θ and q_v is derived from radiosonde measurements; $q_{i/l}$ is provided by the ShupeTurner data set.

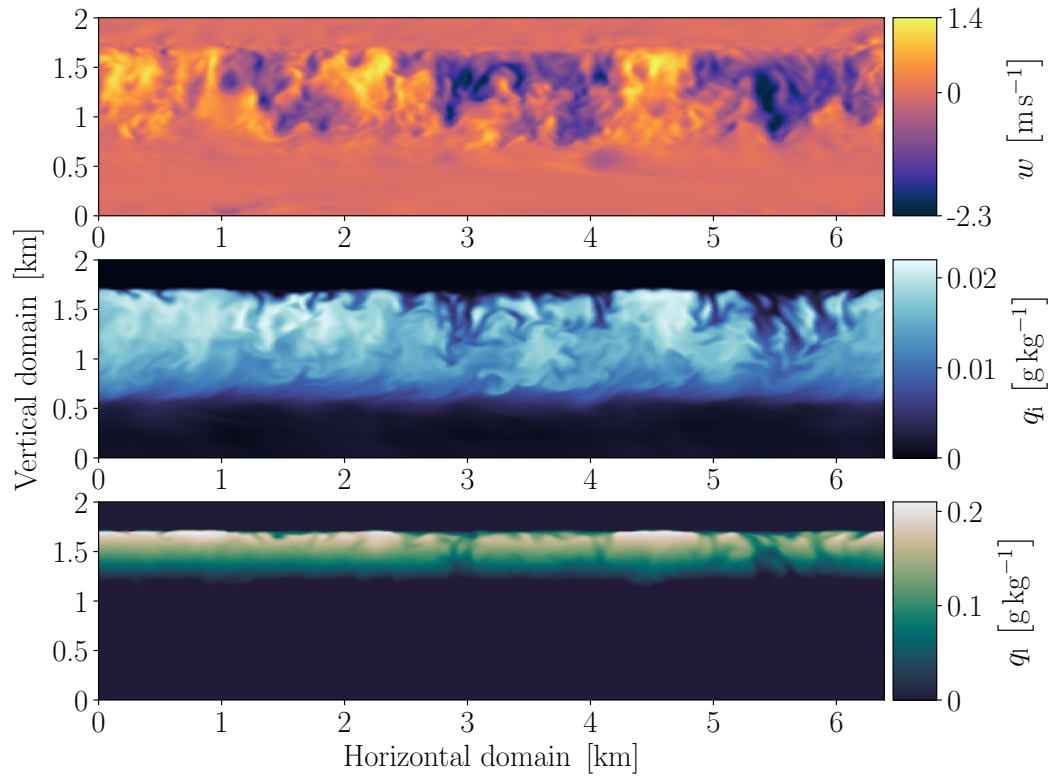


Figure 10. *20191101*: Cross-section plots of vertical velocity w , liquid specific humidity q_l and ice specific humidity q_i . The model output after 1.5 h is shown.

794 4 Discussion

795 In the creation of the year-long library of daily LES experiments, some decisions
 796 had to be made about the numerical setup, the inclusion of datasets, and the usage of
 797 various subgrid-scale parameterizations. All of these decisions affect the eventual results
 798 presented and evaluated in the previous section. Gaining insight into these impacts is
 799 part of an overarching objective of this study, which is to assess the feasibility of turbulence-
 800 resolving LES daily for long continuous periods in the Arctic theatre. To our knowledge,
 801 this has not been attempted or achieved before, and can still be considered a "terra incog-
 802 nita" (Wyngaard, 2004). In this section, the impact of various aspects is discussed in more
 803 detail to convey this experience to the scientific community and inform possible future
 804 efforts of a similar nature.

805 *Grid and domain* Existing limitations in computational resources put limits on
 806 the feasible domain size, grid size, and spatial resolution of LES. This becomes even more
 807 pressing when a high number ($\sim 10^2$) of experiments is to be performed. The first step
 808 was to adopt a vertically telescoping grid, as described in Section 2.3.1. For the PRO-
 809 DUCATION runs the horizontal domain size of $6.4\text{ km} \times 6.4\text{ km}$ was chosen, considered large
 810 enough to contain smaller mesoscale features but small enough to allow resolutions suf-
 811 ficient for resolving Arctic turbulence. A key step that proved crucial for arriving at an
 812 optimized setup was to use small 32×32 horizontal grid simulations for testing early
 813 versions of the model configuration. This was inspired by previous research that adopted
 814 a similar strategy for Arctic LES (Neggers, Chylík, et al., 2019). In Figure 11a this TEST
 815 setup is compared to the PRODUCTION setup in terms of downward longwave radiative
 816 flux. It is evident that the small grid TEST setup, in all its limitations, is still capable
 817 of reproducing year-average radiative climate to a high degree. This suggests good enough
 818 skill to spin up turbulence and maintain liquid clouds, which are reflected in the long-
 819 wave flux. The conclusion from this encouraging result is that using small-grid test se-
 820 tups to develop, calibrate, and optimize full LES runs in the Arctic can be effective, not
 821 just scientifically but also economically, in terms of reducing computational cost and turnover-
 822 time of numerical experiments.

823 *Representation of the surface* The representation of the surface significantly af-
 824 fects the simulations. To achieve a workable experimental setup, a few simplifications
 825 were made. First, the surface is assumed to be homogeneous, a strong simplification in
 826 a region with a notoriously heterogeneous topography (Castellani et al., 2014; Mchedlishvili
 827 et al., 2023). The sea ice surface is often covered by snow, acting as an insulator and as
 828 a source of blowing ice crystals (Wagner et al., 2022) and a variety of aerosols (Held et
 829 al., 2011; Park et al., 2019). While acknowledging these impacts, limitations in data avail-
 830 ability on these aspects motivated our decision not to represent them in the control setup.
 831 Instead, as a guiding principle, observational data was integrated on only three key sur-
 832 face variables; skin temperature, roughness, and albedo. Open-water effects are included
 833 by adapting the skin temperature and humidity to the sea-ice fraction. Figure 11b demon-
 834 strates the beneficial impact of integrating the locally observed surface skin temperature
 835 as measured at the *MetCity* site instead of using *ERA5* reanalysis data. The in-situ ob-
 836 servations are more precise in time and space for the acute situation around the *Polarstern*,
 837 and remove most of the spread introduced by the *ERA5* values. Further, the reanaly-
 838 sis values introduce a known well-defined warm bias for colder surface skin temperatures
 839 (Herrmannsdörfer et al., 2023). This is evident from the positive shift in emitted long-
 840 wave radiation for values $\leq 250\text{ W m}^{-2}$.

841 *Microphysics* In early test simulations, the default *DALES* microphysics scheme
 842 struggled to maintain liquid and frozen cloud mass for conditions below -15°C . A few
 843 microphysical processes were found to cause these issues. As described in Section 2.2.2,
 844 the parameterization for heterogeneous freezing is not valid for those temperature ranges
 845 and had to be limited to the freezing rate for conditions at -15°C . In addition, the max-
 846 imum number concentration for primary ice crystals produced by deposition-nucleation

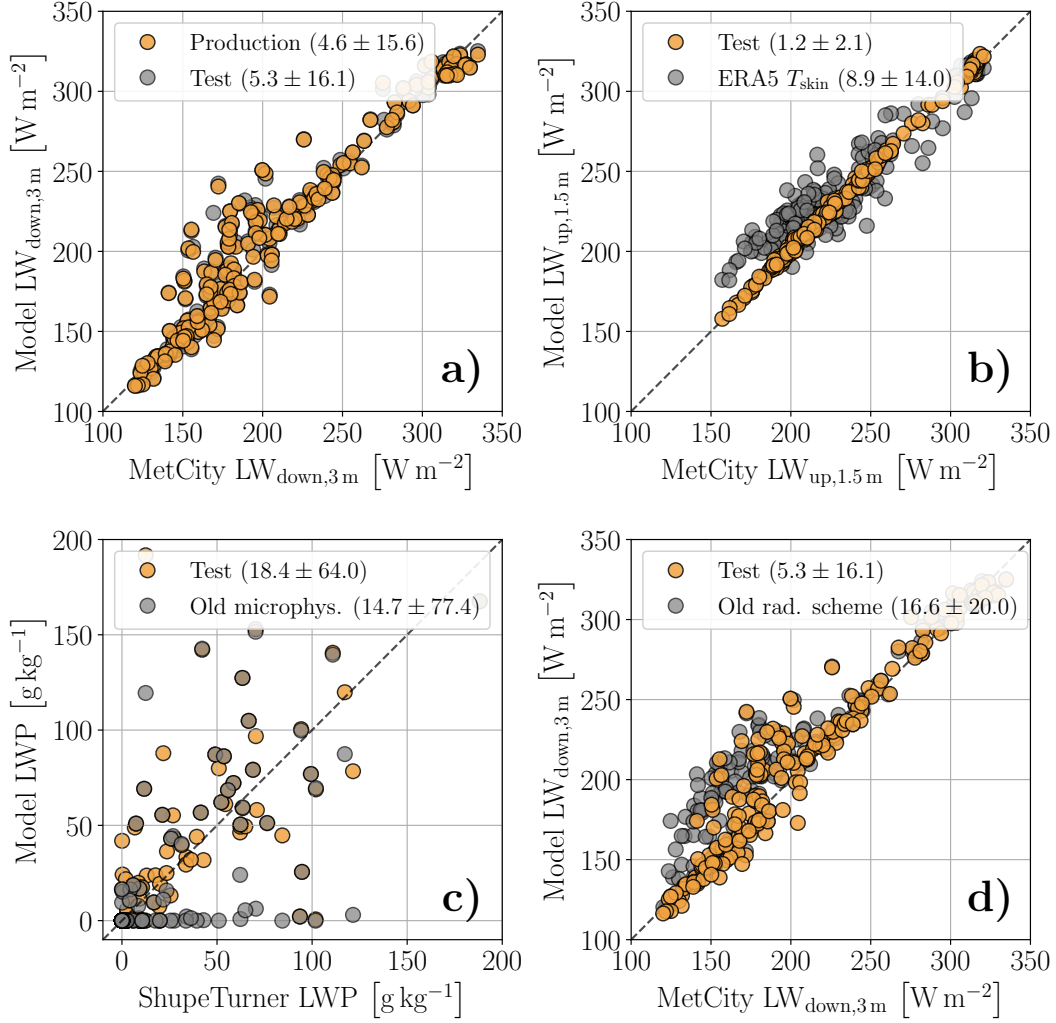


Figure 11. Scatter plots of simulated vs observed variables with different simulation setups. LES results (ordinate) are plotted against *MetCity* (Radiation) or *ShupeTurner* (LWP) measurements (abscissa). Each dot represents a single simulated daily case. The simulations are sampled at $t = 1.5$ h after initialization, the measurements are averaged for 15 min after the radiosonde launch. The dashed line indicates the one-to-one diagonal. Each panel shows the results for two different simulation setups. Panel a) shows the results in downwards longwave radiation for the PRODUCTION and the TEST setup. Analogously, panel b) shows the upwards longwave radiation for the TEST setup and a variation of it with the surface skin temperature derived from *ERA5* data. Panel c) shows the liquid water path for the TEST setup and a variation with the unchanged microphysics scheme. Panel d) shows the downwards longwave radiation for the TEST setup and a variation with the original radiation scheme.

847 is artificially limited to 200 L^{-1} . Figure 11c shows that under cold conditions, the mi-
 848 crophysics scheme in its default setting leads to a full loss of liquid for a significant sub-
 849 set of days, especially for cases with thin ice clouds measured. This loss of liquid stems
 850 from an overestimation of the ice production, quickly depleting any liquid contained in
 851 the column. Introducing the mentioned fixes in the microphysics scheme enabled real-

852 istic simulations of mixed-phase clouds throughout the year, including the Arctic win-
 853 ter.

854 *Ice-radiation interaction* Another key step towards a realistic simulation of ice
 855 clouds was to separate the treatment of liquid and frozen cloud mass in the radiation scheme.
 856 The default *DALES* radiation scheme treated all cloud mass in the same way, a crude
 857 simplification that was abandoned for the final set of runs. Figure 11d compares the near-
 858 surface longwave downward radiation between the original and adjusted radiation scheme,
 859 using the TEST setup. Adding separate ice-radiation interaction reduces the mean bias
 860 towards higher emissions for colder atmospheres with the default scheme, in particular
 861 in the presence of ice clouds, discussed in section 3.2.1. The adjustment does not com-
 862 pletely remove the bias. Note, that the cause of this bias seems to stem from exceeding
 863 the parameterization limits, but the cause for the large radiative effective radius of the
 864 ice crystals might be twofold. Firstly, the ice crystals might be larger than the limits of
 865 the radiations scheme (Ryan, 2000), but secondly, the effective radiative diameter of non-
 866 spherical ice particles depends on the distribution of particle shapes (Fu & Liou, 1993;
 867 Yang & Fu, 2009; Eichler et al., 2009; Mitchell et al., 2011). In 2.2.3 it is assumed that
 868 the mean particle radius calculated by the bulk microphysics scheme can be used with
 869 proportional ratio 1 as the radiative effective radius in the radiation scheme. The result-
 870 ing bias in the longwave radiation statistics indicates that this assumption is not fully
 871 correct. Improving the approximations of ice-cloud radiation emission and their depen-
 872 dence on the distribution of crystal size and shapes is a goal for future research (Ham
 873 et al., 2017; Cairo et al., 2023). These results suggest that the unique impact of ice clouds
 874 on radiative transfer can not be ignored, and should be accounted for in model studies
 875 of the Arctic climate system. This is in agreement with studies of climate models (Waliser
 876 et al., 2011; Fan et al., 2023) that also conclude that further research is required to fully
 877 understand and address these shortcomings (Wang et al., 2020).

878 *Other impacts* Other aspects of the experimental setup might have a significant
 879 impact but are not discussed here for the sake of brevity. These include the treatment
 880 of other relevant microphysical processes, aerosol, and the profiles of cloud liquid and
 881 ice water content used for model initialization. Investigation of these impacts is ongo-
 882 ing, making use of targeted sensitivity experiments from the library of control runs as
 883 described in this study.

884 5 Summary, Conclusions and Outlook

885 This study presents a year-long library of daily high-resolution large-eddy simu-
 886 lations (LES) of the atmospheric boundary layer as observed during the recent *MOSAIC*
 887 drift campaign in the central Arctic. A specific target is to deeply integrate a multitude
 888 of measurements into the experimental configuration. A dedicated standardized model
 889 setup for Arctic conditions is developed and employed for this purpose. An overarching
 890 science objective is to provide a virtual domain with resolved small-scale turbulence and
 891 clouds, which can help in interpreting local measurements made at the *Polarstern* and
 892 *MetCity*. To achieve the desired model skill, various sub-grid parameterizations in the
 893 LES code for microphysical processes and cloud-radiative interaction had to be adapted
 894 to satisfactorily work under central Arctic conditions. The production runs are statis-
 895 tically evaluated against a year of *MOSAIC* data. Three individual case studies are in-
 896 vestigated more closely, to assess the model’s ability to represent key boundary-layer fea-
 897 tures including vertical structure and inversions, mixed-phase clouds, and turbulence.
 898 The impact of various key aspects of the model and experimental setup is assessed.

899 The main scientific conclusions coming out of this research can be itemized as fol-
 900 lows:

- 901 • The statistical evaluation of the library of LES runs demonstrates a generally sat-
902 isfactory performance under a broad range of meteorological conditions concern-
903 ing the surface radiative fluxes, the surface sensible heat flux, near-surface mete-
904 orology, and mixed-phase clouds.
- 905 • The bimodality in the net longwave surface flux typical of the Arctic is well re-
906 produced, with a slight underestimation of intermediate states.
- 907 • A weak overestimation of downward longwave radiation under ice clouds is iden-
908 tified, which is traced to artificial parametric limitations on the maximum effec-
909 tive diameter of ice crystals.
- 910 • Downward shortwave radiation during polar day is slightly underestimated and
911 speculated to be related to the use of one-dimensional radiative transfer in the model.
- 912 • On occasion the surface sensible heat flux, which is an interactive lower bound-
913 ary condition in the simulations, is underestimated.
- 914 • Integrating a multitude of *MOSAiC* data into the initial- and boundary conditions
915 proved crucial for achieving a good statistical agreement. This in particular ap-
916 plies to surface data, sonde data, and value-added cloud products.
- 917 • The detailed investigation of three case studies suggests that initialized liquid and
918 ice cloud layers are maintained long enough to survive in the simulations, reflect-
919 ing that cloud-radiation-turbulence interactions are well captured in this setup.
- 920 • Small grid test simulations are shown to be a viable tool for configuring and op-
921 timizing full grid LES experiments of Arctic boundary layers.

922 The obtained results, and the library of high-resolution turbulence-resolving nu-
923 merical experiments itself, create new research opportunities but also raise some new sci-
924 ence questions. An obvious new scientific opportunity is to use the simulations to gain
925 insight into Arctic Amplification at a process level. The three-dimensional model out-
926 put at high frequencies allows for the sampling of aspects of small-scale physics and dy-
927 namics that are still impossible to measure. A prime example relevant for Arctic climate
928 change is the sampling of tendencies of all terms in the energy and water budgets of the
929 Arctic boundary layer and the surface. Targeted perturbation experiments can be con-
930 ducted to test hypotheses, such as the role of small-scale physical processes in climate
931 feedback mechanisms. The first results of a boundary-layer budget analysis based on the
932 LES dataset for *MOSAiC* as presented in this study was recently published by Linke et
933 al. (2023).

934 Concerning the LES experiments, the library could still be expanded significantly;
935 only $\sim 25\%$ of radiosonde launches were used. Applying the standardized setup to gen-
936 erate more simulations at other sonde launch times is straightforward. While this would
937 represent a significant computational effort, the benefit would be an improved sample
938 size of meteorological conditions throughout the year. The range of observational data
939 sets integrated into the LES experiments could also still be expanded, which might fur-
940 ther improve model skills. In addition, for various already integrated datasets alterna-
941 tive products could be used. Assessing the impact of these actions is a future research
942 topic, and could further inform subsequent high-resolution model efforts of a similar na-
943 ture in the Arctic.

944 In this study, the model evaluation was limited to a few key *MOSAiC* datasets, se-
945 lected based on relevance but also on availability for the full drift. More such products
946 are available; in addition, a great number of special measurements are only available for
947 short intensive observation periods. These include tethered balloon data (Lonardi et al.,
948 2022; Akansu et al., 2023; Pilz et al., 2023), unmanned aerial vehicle (UAV) measure-
949 ments (Egerer et al., 2023; de Boer et al., 2022), among others. The numerical exper-
950 iments for these periods can play a role in providing context for these observational datasets
951 in terms of small-scale variability surrounding the sites. Conversely, these dedicated spe-
952 cial observations can also be used to evaluate the simulations, for example on resolved
953 processes such as turbulence, cloud microphysics, aerosol, and their interactions.

954 A significant part of the work behind this study went into deriving adequate forc-
 955 ing datasets. The content and format of these daily forcings conform to the input require-
 956 ments of most single-column models. A good example is the horizontal homogeneity of
 957 forcing profiles. With resolved LES results now available to accompany these forcings,
 958 and in combination with the extensive *MOSAIC* dataset, this creates a rich testing ground
 959 for improving larger-scale weather and climate models in the central Arctic. The option
 960 exists to test such models for both the whole drift or for a subset of days, to gain fur-
 961 ther process-level understanding and inform parameterization improvement.

962 6 Data availability

963 One of the key objectives of this work is to make all the created data available. The
 964 model code, input, and configuration, the generated forcing files, and the selected model
 965 output can be found at doi.org/10.5281/zenodo.10491362. The forcing files are compat-
 966 ible with typical single-column model (SCM) forcings because *DALES* is run with hor-
 967 izontally homogenous initial- and boundary conditions. The standard model output con-
 968 tains extensive data averaged in space and time. Some output is also available as three-
 969 dimensional fields. For a more detailed description, please refer to the accompanying doc-
 970 umentation. Additional output can always be generated. Please get in touch if needed
 971 for your research. Finally, the *DALES* version used for the final runs is 4.3 with an ex-
 972 tension for mixed-phase microphysics. The specific version used for this work is uploaded
 973 under the link above. For the official *DALES* repository please refer to <https://github.com/dalesteam/dales>.
 974 The combination of forcing files and simulation framework makes the results fully repro-
 975 ducible.

976 Appendix A Vertical grid

In this section the choice of the vertical grid is detailed. The heights of vertical lev-
 els of the grid are calculated as follows:

$$\Delta z^k = \begin{cases} \Delta z_{\text{Start}}, & \text{if } k \leq k_T \\ \Delta z_{\text{Start}} \cdot (1 + s)^{k-(k_T+1)}, & \text{if } k_M > k > k_T \\ \Delta z_{\text{End}}, & \text{if } k \geq k_M \end{cases}$$

$$z^k = \begin{cases} z^{k-1} + \Delta z^k, & \text{if } k > 1 \\ \frac{\Delta z_{\text{Start}}}{2}, & \text{if } k = 0 \end{cases}$$

$$k_T = 120, \quad s = 0.0125, \quad \Delta z_{\text{Start}} = 10 \text{ m},$$

$$k_M = 260, \quad \Delta z_{\text{End}} = 185 \text{ m}$$

977 This produces a grid with a maximum height of 11 857.23 m. The lower 1.2 km are re-
 978 solved with a fixed grid spacing of 10 m. From there, the grid spacing expands accord-
 979 ing to the given formula until it reaches $\Delta z_{\text{max}} = 185 \text{ m}$ at around 7 km height. From
 980 there the grid spacing is kept fixed again until the top of the domain. Figure A1 shows
 981 the height and grid spacing depending on the grid point.

982 Appendix B Radiosonde data

The radiosonde variables (Dahlke et al., 2023) used here are the height z , pressure
 p , temperature T , and the relative humidity RH. From these Θ_v and q_v are calculated

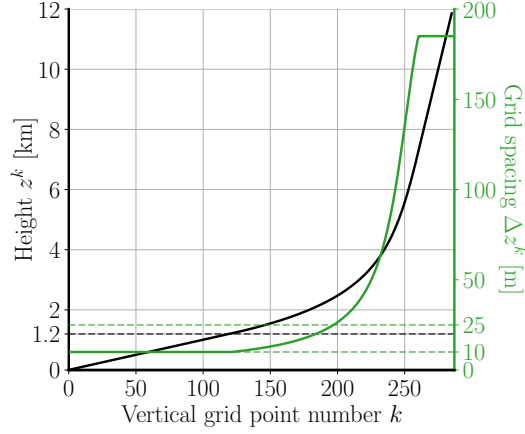


Figure A1. Vertical grid height and spacing of the standardized simulation setup.

using Tetens formula (Tetens, 1930; Murray, 1967):

$$\Theta = T \cdot (p_{\text{ref}}/p)^{R_d/c_p} \quad (\text{B1})$$

$$e_{\text{sat},l} = e_{\text{sat},0} \cdot \exp [a_t \cdot (T - T_m)/(T - b_t)] \quad (\text{B2})$$

$$q_{\text{sat},l} = \frac{R_d/R_v \cdot e_{\text{sat},l}}{p - (1 - R_d/R_v) \cdot e_{\text{sat},l}} \quad (\text{B3})$$

$$q_v = \text{RH} \cdot q_{\text{sat},l} \quad (\text{B4})$$

$$\Theta_v = \Theta \cdot (1 + 0.61 \cdot q_v) \quad (\text{B5})$$

983 Here, $a_t = 17.27$ (dimensionless) and $b_t = 35.86$ K are dimensionless parameteriza-
 984 tion constants, $e_{\text{sat},0} = 610.78$ Pa the reference vapor pressure constant, $R_d = 287.04$ J kg⁻¹ K⁻¹
 985 and $R_v = 461.5$ J kg⁻¹ K⁻¹ the gas constants for dry air and water vapor, $c_p = 1004$ J kg⁻¹ K⁻¹
 986 the specific heat capacity, $T_m = 273.16$ K the melting temperature of ice and $p_{\text{ref}} =$
 987 1000 hPa the reference pressure. Θ is the potential temperature, e_{sat} the saturation wa-
 988 ter vapor pressure with respect to liquid and q_{sat} the corresponding saturation specific
 989 humidity.

A further correction to the derived sonde water vapor specific humidity (q_v) pro-
 file is made: Thin, high-level ice clouds frequently occur in the Arctic atmosphere - in
 areas where the air is saturated with water vapor concerning ice. Small measurement
 uncertainties can lead to situations where $q_v > q_{\text{sat},i}$ and therefore place unrealistic amounts
 of cloud ice in the simulation domain. This is prevented by setting

$$q_v(z) = \min [q_{\text{sat},i}(z), q_v(z)], \quad \text{for } z \geq z_{\text{cut}} \quad (\text{B6})$$

Here, $q_{\text{sat},i}$ is the saturation vapor pressure concerning ice calculated analogously to equa-
 tion (B2) and (B3) with $a_{t,i} = 21.8746$ and $b_{t,i} = 7.66$ K. The cutoff length z_{cut} is cho-
 sen to divide the vertical domain into areas of turbulent ice production in the bound-
 ary layer (e.g., in mixed-phase clouds) and areas of deposition ice production. It is cal-
 culated as the layer of the highest occurring liquid water content q_l above a threshold:

$$z_{\text{cut}} = \max_z \{z \mid q_l(z) \geq 0.01 \text{ g kg}^{-1}\} \quad (\text{B7})$$

990 Here, q_l is derived as described in section 2.3.2.

991 Appendix C Evaluation point

992 To ensure comparability between all cases, a common point in time to evaluate the
 993 simulations has to be found. Different issues have to be considered: First, the grand goal

994 of this work is to be able to compare the simulations to *MOSAIC* measurements. The
 995 initial conditions are derived once at the start of the simulation and, besides weak nudg-
 996 ing, do not influence the further evolution of the atmosphere in the virtual domain. Nat-
 997 urally, after some time, the conditions will have changed so much due to internal tur-
 998 bulent, radiative, and microphysical processes that there is no value in comparing the
 999 LES to the measurements anymore. This motivates an early time point for evaluation.
 1000 But, it has to be considered that the simulation needs time to "spin up". Initially, all
 1001 variables in the LES are homogeneously distributed in the horizontal directions. Their
 1002 vertical distribution and wind lead to turbulent mixing in the domain, ultimately creat-
 1003 ing a realistic spatial distribution of the prognostic variables.

1004 Quantifying the right point in time, considering both of these issues, is difficult to
 1005 achieve since the atmospheric state varies strongly from case to case. Figure C1 shows
 1006 the distribution of the absolute change in total turbulent kinetic energy (TKE) in the
 1007 collection of cases dependent on time. For better comparison, the values are normalized
 1008 by the average value in the shown interval. Generally speaking, the spin-up phase is as-
 1009 sociated with a quick change in TKE, since turbulent processes are still developing. A
 1010 small change in TKE signifies a period of quasi-equilibrium, where the state of the at-
 1011 mosphere is not shifting significantly. Therefore, the point in time for the evaluation of
 1012 the simulations is chosen to be 1.5 h, around the general minimum of change in TKE.

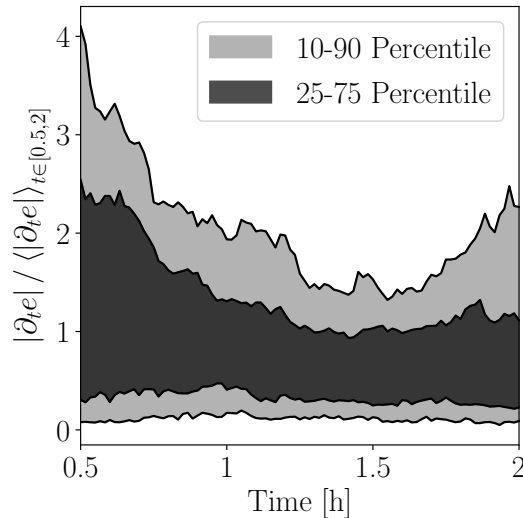


Figure C1. Distribution of normalized absolute change in total turbulent kinetic energy of all simulated cases depending on simulation time.

1013

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1022 Hersbach et al. (2018a, 2018b) was downloaded from the Copernicus Climate Change
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