# An evaluation of kilometer-scale ICON simulations of mixed-phase stratocumuli over the Southern Ocean during CAPRICORN

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#### Abstract

This study investigates the representation of stratocumulus (Sc) clouds, cloud variability, and precipitation statistics over the Southern Ocean (SO) to understand the dominant ice processes within the Icosahedral Nonhydrostatic (ICON) model at the kilometer scale using real case simulations. The simulations are evaluated using the shipborne observations as open-cell stratocumuli were continuously observed during two days (26th -27th of March 2016), south of Tasmania. The radar retrievals are used to effectively analyze the forward-

simulated radar signatures from Passive and Active Microwave TRAnsfer (PAMTRA). We contrast cloud-precipitation statistics, and microphysical process rates between simulations performed with one-moment (1M) and two-moment (2M) microphysics schemes. We further analyze their sensitivity to primary and secondary ice-phase processes (Hallett–Mossop and collisional breakup). Both processes have previously been shown to improve the ice properties of simulated shallow mixed-phase clouds over the SO in other models. We find that only simulations with continuous formation, growth, and subsequent melting of graupel, and the effective riming of in-cloud rain by graupel, capture the observed cloud-precipitation vertical structure. In particular, the 2M microphysics scheme requires additional tuning for graupel processes in SO stratocumuli. Lowering the assumed graupel density and terminal velocity, in combination with secondary ice processes, enhances graupel formation in 2M microphysics ICON simulations. Overall, all simulations capture the observed intermittency of precipitation irrespective of the microphysics scheme used, and most of them sparsely distribute intense precipitation (>1m h-1) events. Furthermore, the simulated clouds are too reflective as they are optically thick and/or have high cloud cover.

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#### Key Points:

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13	•	The continuous formation, in-cloud layer growth by riming, and sub-cloud layer melt-
14		ing of graupel are crucial to represent observed Southern Ocean stratocumulus cloud-
15		precipitation structures during CAPRICORN.
16	•	Boundary layer decoupling is reasonably captured in km-scale simulations when the
17		positive bias in the prescribed ERA5 SST is removed.
18	•	During CAPRICORN 2016, graupel melting is the predominant rain source in South-

• During CAPRICORN 2016, graupel melting is the predominant rain source in South ern Ocean stratocumuli as simulated in ICON.

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#### 20 Abstract

This study investigates the representation of stratocumulus (Sc) clouds, cloud variability, 21 and precipitation statistics over the Southern Ocean (SO) to understand the dominant ice 22 processes within the Icosahedral Nonhydrostatic (ICON) model at the kilometer scale us-23 ing real case simulations. The simulations are evaluated using the shipborne observations 24 as open-cell stratocumuli were continuously observed during two days (26<sup>th</sup>-27<sup>th</sup> of March 25 2016), south of Tasmania. The radar retrievals are used to effectively analyze the forward-26 simulated radar signatures from Passive and Active Microwave TRAnsfer (PAMTRA). We 27 contrast cloud-precipitation statistics, and microphysical process rates between simulations 28 performed with one-moment (1M) and two-moment (2M) microphysics schemes. We further 29 analyze their sensitivity to primary and secondary ice-phase processes (Hallett-Mossop and 30 collisional breakup). Both processes have previously been shown to improve the ice proper-31 ties of simulated shallow mixed-phase clouds over the SO in other models. We find that only 32 simulations with continuous formation, growth, and subsequent melting of graupel, and the 33 effective riming of in-cloud rain by graupel, capture the observed cloud-precipitation ver-34 tical structure. In particular, the 2M microphysics scheme requires additional tuning for 35 graupel processes in SO stratocumuli. Lowering the assumed graupel density and terminal 36 velocity, in combination with secondary ice processes, enhances graupel formation in 2M mi-37 crophysics ICON simulations. Overall, all simulations capture the observed intermittency 38 of precipitation irrespective of the microphysics scheme used, and most of them sparsely 39 distribute intense precipitation  $(>1 \,\mathrm{mm}\,\mathrm{h}^{-1})$  events. Furthermore, the simulated clouds are 40 too reflective as they are optically thick and/or have high cloud cover. 41

#### 42 Plain Language Summary

Stratocumulus (Sc) clouds cover a large portion of the Southern Ocean (SO), where 43 they substantially cool the ocean surface. Our understanding of the complex physics of these 44 clouds, which include both liquid and ice remains incomplete, and hence the representation 45 of these clouds in global climate and weather models remains biased. In particular, their 46 timing, frequency of occurrence, cloud phase and distribution, cloud cover, and precipitation 47 characteristics are still associated with open research questions. This results in SO radiative 48 biases and increased uncertainty for estimating climate sensitivity. We use the measurements 49 from the Clouds, Aerosols, Precipitation, Radiation, and atmospherIc Composition Over the 50 southeRn oceaN (CAPRICORN) voyage south of Tasmania, to evaluate the representation 51 of broken cloud fields, the dominant ice processes, and the precipitation characteristics in 52 the high-resolution numerical simulations. Our results suggest that, in addition to capturing 53 the observed discrete cloud events, the graupel formation, its growth in the cloud layer, and 54 subsequent melting in the sub-cloud layer are critical processes in accurately representing 55 the SO broken Sc fields and precipitation characteristics during CAPRICORN. Additionally, 56 compared to observations, the simulated clouds are too reflective. 57

#### 58 1 Introduction

The Southern Ocean (SO)  $(45^{\circ}\text{S}-65^{\circ}\text{S}, 180^{\circ}\text{W}-180^{\circ}\text{E})$  is one of the regions with the 59 highest annually-averaged low cloud fraction of 60% (Muhlbauer et al., 2014). The low 60 clouds, in particular, stratocumulus (Sc) clouds are capped by a strong temperature inver-61 sion of 10-20 K in just a few vertical meters at the top of the Sc topped boundary layer 62 (Riehl et al., 1951; Caughey et al., 1982; Bosello et al., 2007). Cloud-top (CT) radiative 63 cooling due to longwave emission is the most crucial mechanism that drives the convective 64 instability to sustain Sc clouds, and further enhances the inversion at the CT. The supply 65 of moisture from the ocean surface by latent heating, cooling from evaporation and subli-66 mation in the sub-cloud layer (cold pool generation), the associated large-scale turbulent 67 eddies, entrainment from the free tropospheric atmosphere at the CT, and precipitation are 68 the processes interlinked with the mesoscale variability of Sc clouds (Bosello et al., 2007). 69

Precipitation and albedo strongly depend on the micro- and macrophysical properties, and
 the spatio-temporal distribution of hydrometeors within the Sc cloud field. A numerical
 weather or climate model must capture the aggregated effect of all these complex processes
 which occur at diverse spatial and temporal scales in its grid-scale tendencies and diagnostic
 variables.

A study by Bodas-Salcedo et al. (2012) with the atmosphere-only Met Office model 75 reported that the low and mid-level clouds at the lee of the cold front of cyclones in the SO 76 are responsible for the downwelling SW positive bias. The representation of Sc clouds largely 77 differs in the 6<sup>th</sup> Coupled Model Intercomparison Project (CMIP6) compared to CMIP5 78 (Schuddeboom & McDonald, 2021). The SO Sc clouds were too few and too bright in 79 CMIP5, whereas they occur more often in CMIP6, and are not brighter compared to Clouds 80 and the Earth's Radiant Energy System (CERES) data. While a correct representation 81 of cloud macrophysics alone is not a sufficient criterion, a better representation of cloud 82 microphysics is essential for addressing the SW bias (Fiddes et al., 2022). The microphysics 83 parameterization controls the shape, size, and concentration of liquid and ice hydrometeors 84 in the SO Sc mixed-phase clouds (MPCs, and which strongly influence the cloud radiative 85 effect. 86

Many models underestimate the presence of supercooled liquid water (SLW), since ice 87 grows at the expense of liquid water in MPCs when the ambient vapor pressure is subsatu-88 rated and supersaturated with respect to liquid and ice respectively (termed as the Wegener-89 Bergeron-Findeisen process). The deficiency of the models in simulating supercooled liquid 90 in SO MPCs can be compensated by slowing down the vapor deposition growth rate of ice 91 crystals. This can be achieved by modifying the shape parameter of ice crystals. Although 92 the focus is the SO, this has an impact on the liquid water content in either hemisphere 93 (Varma et al., 2020). The ice formation process in mixed-phase Sc clouds is poorly under-94 stood (Fridlind et al., 2007), and the ice crystal number concentration (ICNC) is one of the 95 largest uncertainties in these SO clouds. Heterogeneous nucleation requires ice nucleating 96 particles (INPs) for droplet freezing where SLW prevails in metastable equilibrium. Never-97 theless, the SO is a remote region with very low INP concentrations. For example, INP con-98 centrations of 0.38 to 4.6 m<sup>-3</sup> were observed at -20°C during March-April 2016 (McCluskey 99 et al., 2018). The sparse INPs in SO limit droplet freezing and further the production of ice 100 crystals, resulting in reduced precipitation and brighter clouds (Vergara-Temprado et al., 101 2018). However, a higher ICNC than INP concentration was observed during an earlier SO 102 campaign. This was associated with the secondary ice production processes (Huang et al., 103 2017). The rime splintering process by Hallett and Mossop (1974), or HM, a predominant 104 secondary ice production process in global climate models, is insufficient to account for the 105 observed ICNC. The deficiency in the modeled ICNC in this remote atmosphere can be 106 better described by HM in conjunction with collisional breakup processes (Sotiropoulou et 107 al., 2020). 108

The objective of this paper is to investigate the significance of ice processes and the 109 associated precipitation, and to understand the dominant microphysical processes in mixed-110 phase open-cell stratocumuli using numerical simulations. In this study, we evaluate the 111 kilometer-scale ICON-NWP (Icosahedral Nonhydrostatic – Numerical Weather Prediction) 112 simulations with the shipborne in-situ and remote sensing observations obtained during 113 Clouds, Aerosols, Precipitation, Radiation, and atmospherIc Composition Over the south-114 eRn oceaN (CAPRICORN) on 26<sup>th</sup>-27<sup>th</sup> of March 2016, south of Tasmania. Among the 115 numerous observations, a suite of instruments measured the cloud and precipitation char-116 acteristics, boundary layer structure, and surface energy fluxes during this first voyage of 117 CAPRICORN (Mace & Protat, 2018a, 2018b). A set of convection-permitting simulations 118 (referred to as "kilometer-scale") are performed in this study. The kilometer-scale simu-119 lations with active shallow-convection parameterization are used to address the following 120 research questions in this study. 121

- How well do kilometer-scale ICON simulations capture the vertical structure of postfrontal mixed-phase cloud-precipitation in SO?
   How do different ice-phase processes impact precipitation formation in observed and
  - simulated mesoscale cellular convective (MCC) clouds during CAPRICORN?
  - Are these conclusions robust across different microphysics schemes of varied complexity available within ICON?

#### <sup>128</sup> 2 Observations, Simulations, and Analysis Methods

129 2.1 Observations

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The CAPRICORN voyage I took place south of Tasmania from the 13<sup>th</sup> of March 2016 130 to the 15<sup>th</sup> of April 2016. During this time a consistent period of post-frontal open MCC 131 clouds was observed between 26<sup>th</sup> and 27<sup>th</sup> of March 2016. The time period is characterized 132 by a high-pressure system of  $1030 \,\mathrm{hPa}$  located south-west of Australia on the  $26^{\mathrm{th}}$  of March 133 2016 (Figure 1a). A long cold front that stretches from  $38^{\circ}S-60^{\circ}S$ , which is associated with 134 the high-pressure system, passed the ship on  $25^{\text{th}}$  of March 2016 and Tasmania on  $26^{\text{th}}$  of 135 March 2016. Open MCC clouds were observed for 36 hours at the lee of the cold front 6 136 hours later of its transit, followed by closed MCC clouds later on (Lang et al., 2021). Char-137 acterizing the clouds and precipitation properties and examining their occurrence statistics 138 were part of the objective of the CAPRICORN field study using modern in-situ and remote 139 sensing instruments aboard the R/V Investigator. A comprehensive overview of all instru-140 ments is provided in Mace and Protat (2018a, 2018b). Here, we only focus on measurements 141 and retrievals relevant for this study. 142

The thermodynamic profiles of the atmosphere are obtained from radiosondes on  $26^{\text{th}}$ 143 of March 2016 at 01:42:00 UTC and 06:24:00 UTC. The intensities of precipitation are ob-144 served from Ocean Rain and Ice-Phase Precipitation Measurement Network (OceanRAIN) 145 disdrometer (Klepp, 2015). The downwelling SW radiation is measured from Precision 146 Spectral Pyranometer (PSP) at the port and starboard sides of the R/V Investigator. 147 The cloud-precipitation vertical structure is characterized by a 95-GHz single-polarization 148 Bistatic Radar System for Atmospheric Studies (BASTA) Doppler cloud radar with a verti-149 cal resolution of 25 m and temporal resolution of 12 s (Delanoë et al., 2016). The cloud base 150 phase (CBP) and the cloud base height (CBH) are derived from a 355 nm cloud-aerosol 151 Leosphere RMAN-511 mini-Raman lidar with a vertical resolution of 15 m and temporal 152 resolution of 35s (Royer et al., 2014). The SST is measured from an in-situ instrument 153 (which was the source of the sea surface temperature (SST) bias - see section 2.2.3) mea-154 sures. The combined radar and lidar data (termed as the radar-lidar merged product) with 155 a vertical resolution of 25 m and temporal resolution of 1-min is used to determine cloud 156 phase. Temperature from the ERA-interim reanalysis is interpolated onto the pixels of the 157 radar-lidar merged product. At sub-freezing temperatures, each pixel is classified as (a) 158 SLW if only lidar signal is detected, (b) mixed-phase if lidar and radar signals are detected, 159 and (c) mixed-phase or ice-phase if only a radar signal is present (Noh et al., 2019). The 160 layer integrated lidar backscatter and lidar depolarization ratio ( $\delta$ ) are used (see section 2.3) 161 for details) to determine CBH and CBP (Hu et al., 2009, 2010; Alexander & Protat, 2018; 162 Mace & Protat, 2018a). 163

#### <sup>164</sup> 2.2 Simulations

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#### 2.2.1 Model Setup

Real case simulations are performed with ICON-NWP. The initial and hourly lateral boundary conditions are derived from the European Centre for Medium-Range Weather Forecasts fifth reanalysis (ERA5). The dynamical downscaling of ERA5 to the kilometer scale is achieved by a two-way nesting strategy (Figure 1b). Across three domains the horizontal resolution is roughly doubled each time from 4.9 km to 2.4 km to the highest



Figure 1: (a) Map of synoptic conditions south of Tasmania on  $26^{\text{th}}$  of March 2016 at 00 UTC. (b) ICON nested domains for simulation, where Domain-1 (outer domain) has 264948 cells with 4.9 km of horizontal resolution, Domain-2 has 304100 cells with 2.4 km of resolution, Domain-3 (highest resolution domain) has 556216 cells with 1.2 km of resolution, and the red line shows the ship track for two days ( $26^{\text{th}}-27^{\text{th}}$  of March 2016).

resolution of  $1.2 \,\mathrm{km}$ . To minimize the numerical error in this study, the two-day (26<sup>th</sup> of 171 March 2016 at 00:00:00 UTC to 28<sup>th</sup> of March 2016 at 00:00:00 UTC - case study period) 172 simulation period was split into two 36 h time periods. The first 12 hours of each simulation 173 are used as spinup. Furthermore, the last 12 hours of the first run (12 UTC of 25<sup>th</sup> of March 174 until 00 UTC of 27<sup>th</sup> of March) overlap with the first 12 hours of the second run (12 UTC of 175 26<sup>th</sup> of March until 00 UTC of 28<sup>th</sup> of March). The model is run with 60 vertical layers and 176 a model top height of  $23 \,\mathrm{km}$ . The layers within the boundary layer are stretched from 20 to 177 200 m in thickness. From Mellor and Yamada (1982), the turbulence scheme developed by 178 Raschendorfer (2001) based on the prognostic turbulent kinetic energy (TKE) equation with 179  $2^{\rm nd}$  order closure on level 2.5 is used. The rapid radiative transfer model (RRTM) developed 180 by (Mlawer et al., 1997) is used for radiation. All convection is parameterized following the 181 approach of Bechtold et al. (2008). In the kilometer-scale resolution domain (1.2 km), only 182 shallow convection is parameterized. Horizontal cloud variability at the kilometer scale was 183 best captured in simulations with parameterized shallow convection, which was thus kept 184 turned on while all other convection parameterizations were turned off. All the runs with 185 this setup are summarized in Table 1. 186

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#### 2.2.2 Microphysics Sensitivity Experiments

The sensitivity of the simulated cloud precipitation and cloud phase statistics are ex-188 plored with respect to two different bulk microphysical schemes. The simpler, and compu-189 tationally more efficient, one-moment (1M) scheme (Doms et al., 2011; Seifert, 2008) runs 190 with fixed assumed number concentrations. Meanwhile a fully prognostic description of 191 both, number and mass - and thus size-, is used in the two-moment (2M) scheme (Seifert 192 & Beheng, 2006). The 1M control simulation (1M.90ND) is performed with a cloud droplet 193 number concentration (CDNC) representative for SO austral conditions. This was deter-194 mined as 90 cm<sup>-3</sup> derived from the combined data of CAPRICORN I, II, and MARCUS 195 (Measurements of Aerosols, Radiation, and Clouds over the Southern Ocean) for the aus-196 tral summer months of November-April (Mace, Protat, et al., 2020). The sensitivity with 197 respect to prescribed CDNC is investigated in an additional run with a lower prescribed 198 CDNC of  $20 \,\mathrm{cm}^{-3}$  (1M.20ND), which is representative for austral autumn observations ob-199 tained during CAPRICORN I (Mace, Benson, & Hu, 2020) and austral winter aircraft ob-200 servations (Ahn et al., 2017). In the 1M microphysics scheme, the ICNC is diagnosed using 201 the temperature-dependent Cooper parameterization (Cooper, 1986), where heterogeneous 202 ice nucleation occurs below a temperature threshold of -5°C. 203

Expt	Expt Name	Equation/Description					
No.							
Bulk	Bulk microphysics sensitivity experiments (Simulation period: 48 hours)						
1	1M 20ND	1M microphysics scheme and CDNC = $20 \text{ cm}^{-3}$					
1	1M OOND	1M microphysics scheme and $CDNC = 20 \text{ cm}^{-3}$					
Δ	(control simulation)	The incrophysics scheme and $CDNC = 90  cm^{-3}$					
2	(control simulation)	2M microphysics scheme and no secondamy ice phase					
3	21 <b>VI.</b> F	2141 Inicrophysics scheme and no secondary ice-phase					
4	9М НМ	2M microphysics scheme with rime splintering sec					
4	2111.11111	and ary ice process					
5	2M HM BR03	2M microphysics scheme with rime splintering and					
0	21111111111111100	collisional breakup (rimed mass fraction is 0.3) sec-					
		ondary ice process					
Micro	physical process sensitivit	ty experiments (Simulation period: 24 hours)					
1111010	physical process sension.	(Simalation period: 2116415)					
1	2M.HM	Default: CCN = $400  cm^{-3}$ ; power-law for v <sub>r</sub> =					
		$95.5616 * exp(0.22 * log(x_r))$ : Ice to snow minimum					
		diameter threshold = $100 \mu m$ ; low graupel density;					
		low graupel velocity; graupel maximum diameter (=					
		$2 \text{ mm}$ ; $v_i = 27.7 * \exp(0.21579 * \log(x_i))$					
2	2M.P	Secondary ice production processes switched off					
3	2M.HM.BR03	Collisional breakup with rimed mass fraction $= 0.3$					
4	CCN10	$CCN = 10  cm^{-3}$					
5	CCN1000	$CCN = 1000  cm^{-3}$					
6	aukcc*0.5	Autoconversion cloud kernel coefficient is reduced by					
		50% (= 0.5*6E2)					
7	aukcc*2	Autoconversion cloud kernel coefficient is doubled (=					
		2.0*6E2)					
8	ice_vel_coef	$v_i = 317 * exp(0.363 * log(x_i))$					
9	$rain_{atlas}$	$v_r = 9.292 - (9.623 * exp(-622.2 * a_geo * exp(b_geo + exp(b_geo + exp(b_geo + exp(b_geo + exp(b_geo + exp(b_geo + exp(-622.2 * a_geo + exp(-622.2 + exp(-622.$					
		$\log(x_r)))$					
10	$agg_50$	Aggregated ice to snow minimum diameter threshold					
		$= 50  \mu m$					
11	$agg_200$	Aggregated ice to snow minimum diameter threshold					
		$= 200 \mu m$					
12	gr_d_m	$d_g = 0.3456 * x_g^{0.5571}$ (Medium lump graupel den-					
10	1.1	sity)					
13	gr_d_h	$d_g = 0.3456 \uparrow x_g^{0.3764}$ (High lump graupel density)					
14	gr_v_h	$v_g = 9.4465 + x_g^{\circ 12}$ (High lump graupel velocity)					
15	gr_max_dia	Graupel maximum diameter increased to $5 \mathrm{mm}$					

Table 1: Bulk microphysics sensitivity experiments for the entire simulation period ( $26^{\text{th}}$  of March 2016 at 00:00:00 UTC to  $28^{\text{th}}$  of March 2016 at 00:00:00 UTC) and microphysical process sensitivity experiments with 2M microphysics scheme (simulated on  $27^{\text{th}}$  of March 2016). v, terminal velocity of hydrometeors in  $m \, s^{-1}$ ; d, diameter of hydrometeors in m; x, mass of hydrometeors in kg;  $v_{\text{sed.i}}$  is maximum sedimentation velocity of ice; CCN, cloud condensation nuclei; CDNC, cloud droplet number concentration; a\_geo and b\_geo constants in rain hydrometeor mass - fall speed relation; subscripts r, i and g represent rain, ice and graupel respectively.

To better understand the significance of ice processes in SO mixed-phase Sc clouds, sensitivity experiments were carried out with the 2M scheme since it has control over CCN and INP specifications. The cloud-precipitation vertical structure and the precipitation statistics as the result of cloud ice processes are studied using sensitivity experiments: 2M.P, 2M.HM, and 2M.HM.BR03 described in Table 1. The collisional breakup parameterization developed

by Phillips, Yano, and Khain (2017); Phillips, Yano, Formenton, et al. (2017) based on the 209 principle of ejected fragments as a function of the initial collisional kinetic energy of solid 210 hydrometeors is implemented for ice, snow and graupel in ICON. The parameterization of 211 prognostic CDNC is adapted from Segal and Khain (2006) and the prognostic ICNC from 212 Seifert and Beheng (2006). The activation scheme for CDNC is computed for a prescribed 213 lognormal aerosol size distribution with a mean number concentration of  $400 \,\mathrm{cm}^3$  and a 214 mean radius of  $0.04 \,\mu m$  (see supporting information S2). Immersion freezing for sea spray 215 aerosols is parameterized by McCluskey et al. (2018) and dust aerosol by Demott et al. 216 (2015); McCluskey et al. (2019). These adjustments to the default heterogeneous freezing 217 parameterization Seifert and Beheng (2006) were performed to better capture the remote 218 aerosol environment of the SO relevant for INP nucleation. A fictitious increase of the po-219 tential INPs at low temperatures was avoided by relaxing INP concentrations exponentially 220 with height over 4 km. Immersion freezing rates are limited to temperatures at or below 221 -5°C. A small perturbed physical parameter ensemble is performed for 2M simulations for a 222 range of parameters related to the simulated graupel budget (G\_budget) in SO stratocumuli. 223 In addition to dynamics, the formation and depletion of graupel is based on the sensitivity 224 of the interlinked microphysical processes. The impact of various factors that can influence 225 these microphysical processes and further the G<sub>-</sub>budget is analyzed (microphysical process 226 sensitivity experiments in Table 1). 227

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#### 2.2.3 SST Bias Correction

During CAPRICORN, the instruments for measuring SST were at the ship deck from 229 22<sup>th</sup>-26<sup>th</sup> of March 2016. This biased the assimilation of SST in ERA-Interim, ERA5, and 230 MERRA-2 products by up to 6°C (Lang et al., 2021). This artificially increases the sea-air 231 temperature differences, which may have an impact on surface cold pools, boundary layer 232 decoupling, and the average inversion height. Hence, we corrected the bias by limiting the 233 maximum SST to 12°C in the entire simulation domain (Figure S1a). We thus ran the 234 simulations essentially with prescribed SST of  $12^{\circ}$ C along the track. This fix improved the 235 overall match between observed and simulated SST and surface fluxes shown in Fig S1, but 236 fails to capture the  $1-2^{\circ}C$  increase in SST after 36 hours which coincides with the transition 237 of sampling open-cell cloud structures to solid cloud decks towards the end of the 48 hours 238 period (Figure 2a). 239

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#### 2.3 Analysis Methods

Minimum thresholds are applied in the simulations for all hydrometeor categories. 241 These are specified as  $0.01 \,\mathrm{g\,m^{-3}}$  for cloud liquid,  $0.0001 \,\mathrm{g\,m^{-3}}$  for cloud ice, and  $0.00001 \,\mathrm{g\,m^{-3}}$ 242 for rain, snow, graupel, and hail. The simulated cloud-top height (CTH), cloud-top phase 243 (CTP), CBH and CBP are identified based on these thresholds. Two-dimensional field 244 statistics are computed in a clipped zone  $(147^{\circ} > \text{lon} > 143^{\circ}; -44^{\circ} > \text{lat} > -48^{\circ})$  enclosing 245 the ship track. The retrieved CTH along the ship track has been derived from the ground-246 based BASTA radar reflectivity profile. Lidar backscatter is very sensitive to the water 247 droplet population and attenuates completely within a few tens of meters of the cloud. It is 248 thus a reliable measure for identifying the CBH. We cannot use the minimum height of the 249 first backscatter signal of the lidar to determine the cloud base (CB), as this metric may 250 be biased low by precipitation. Instead, the CBH is calculated as the altitude at which the 251 maximum vertical gradient of backscatter occurs. The phase partitioning at the CBH is 252 based on the threshold values for  $\delta$  (ratio of perpendicular to parallel backscatter intensities 253 with respect to the transmitter polarization axis). The depolarization ratio is very small for 254 cloud water and smaller raindrops since the parallel backscatter predominates. Mace and 255 Protat (2018a) suggest  $\delta < 0.02$  for liquid-dominant layers and  $\delta > 0.03$  for ice-dominant 256 layers. We assumed a mixed-phase category in the in-between range. Since lidar backscat-257 ter is influenced by densely populated hydrometeors in the resolution volume, we are more 258 likely to miss the presence of ice at CB. Hence we include an additional criterion one level 259

below the identified CB to correct the CBP as ice-phase if  $\delta \ge 0.03$  and the temperature is less than 3°C. The CB precipitation is calculated as the average precipitation in the lowest one-third of the cloud depth as defined by Wood (2005).

We analyze the microphysical processes with 1M and 2M microphysics schemes to examine the shortcomings in representing the cloud-precipitation vertical structure. The microphysical processes are normalized by the total water vapor loss to the ice-phase (Equation 1) to understand their relative importance, as shown in Equation 2.

$$WVL^{*}(n,k,i) = X^{*}{}_{nuc}(n,k,i) + X^{*}{}_{I\_dep}(n,k,i) + X^{*}{}_{S\_dep}(n,k,i) + X^{*}{}_{G\_dep}(n,k,i) + X^{*}{}_{H\_dep}(n,k,i)$$
(1)

$$\overline{X}(n,k,i) = \frac{\sum_{\substack{n,k,i \\ t,4km,nclip \\ \sum_{n,k,i}}} X^*(n,k,i) V(n,k,i)}{\sum_{\substack{n,k,i \\ n,k,i}} WVL^*(n,k,i) V(n,k,i)}$$
(2)

Here, V is the cell volume (m<sup>3</sup>); WVL<sup>\*</sup> is the total water vapor loss to the ice-phase (kg m<sup>-3</sup> s<sup>-1</sup>); X<sup>\*</sup> is the rate of the mass density for a given microphysical process (kg m<sup>-3</sup> s<sup>-1</sup>); X<sup>\*</sup><sub>nuc</sub>, X<sup>\*</sup><sub>idep</sub>, X<sup>\*</sup><sub>sdep</sub>, X<sup>\*</sup><sub>gdep</sub>, X<sup>\*</sup><sub>hdep</sub> are the rate of mass density of ice nucleation, ice deposition, snow deposition, graupel deposition and hail deposition (kg m<sup>-3</sup> s<sup>-1</sup>) respectively;  $\overline{X}(i,j,k)$  is calculated for a time period t (index n), up to 4 km altitude (index k) and the spatial extent (index i) is clipped around the ship track (nclip:  $147^{\circ} \ge lon \ge 143^{\circ}$ ;  $-44^{\circ} \ge lat \ge -48^{\circ}$ ).

Furthermore, the forward simulated ICON output from the Passive and Active Microwave TRAnsfer (PAMTRA) model (Mech et al., 2020) is evaluated against the BASTA radar retrievals. For evaluating the simulation with CAPRICORN, the mean of the simulated data within 2 km at each coordinate along the ship track is used. The supporting information S1 provides a basic setup of PAMTRA for 1M and 2M simulations.

#### 274 **3 Results**

Cloud and precipitation characteristics during CAPRICORN between the 26<sup>th</sup> and 27<sup>th</sup> 275 of March 2016 have been studied in great detail in Lang et al. (2021). They hypothesized 276 that ice processes could play a significant role in the SO open-cell precipitation during this 277 period. In this section, we use the retrieved cloud properties and precipitation characteristics 278 from the observations to evaluate the skill of kilometer-scale ICON simulations (control 279 simulation). Collected soundings (Figures S2a and S2b) are compared to the simulated 280 soundings in the post-frontal environment of the control simulation (1M.90Nd). Note, that 281 the second sounding is the thermodynamic profile obtained during the open-cell period. 282 While the overall profiles are well captured, the inversion height is underestimated by at 283 least 200 m during the open-cell period (Figure S2b). The transition layer that separates 284 the two observed cloud layers is located at  $1.2 \,\mathrm{km}$  (0.9 km), and  $1.7 \,\mathrm{km}$  (1.8 km) in the 285 first and second observed (simulated) sounding respectively. Although the simulated CTH 286 is underestimated in the second profile, the simulated mean CTH along the ship track is 287 slightly overestimated at 2.2 km as compared to the observed 1.8 km. 288

289

#### 3.1 Evaluation of Cloud-Precipitation Vertical Structure and Statistics

The vertically pointing single-polarization Doppler radar reflectivity is used to evaluate the vertical cloud and precipitation structures. Figure 2a shows that intermittent radar reflectivities occur throughout the two days characterizing sporadic precipitation events.

The increase in reflectivity across the melting layer is caused by the higher reflectivity of 293 liquid hydrometeors than previously frozen hydrometeors (i.e. cloud ice, snow and graupel). 294 The melting of solid hydrometeors produces liquid precipitation of reduced size, which is 295 characterized by a higher terminal fall velocity than ice particles due to an increase in 296 density. This is clearly visible in the more negative Doppler velocities below the melting 297 layer (Figure S3a). Furthermore, this decrease in Doppler velocity across the melting layer is 298 well captured by the simulations. However, the mean Doppler velocity of melted rain seems 299 biased low (falling faster) in 1M.90ND. Furthermore, the presence of ice above the freezing 300 line is further supported by the merged radar-lidar product (Figure 2c). Most streaks (also 301 termed as cloud events) above the melting level are classified as mixed-phase, or consist of 302 adjacent patches of ice and SLW. 303

To understand the formation and evolution of precipitation in the cloud and the cloud-304 precipitation vertical structure, we generate (Figure 2a) a contoured frequency by altitude 305 diagram (CFAD) from the BASTA radar reflectivity retrieval. The CFAD is normalized by 306 the total samples in every reflectivity bin. The numbers at the top of the CFAD denote 307 the number of samples within a reflectivity bin (summed along all altitudes) normalised by 308 the maximum number of samples (summed across all altitudes) in one reflectivity bin found 309 across all reflectivity bins. The CFAD aggregates the cloud-precipitation data of the same 310 reflectivity-height bins across multiple timestamps. Thus a physical relationship between 311 bins across heights may no longer be given. However, a statistical analysis of all observed 312 vertical reflectivity profiles (Figures S4a) which exclude "single data" points ("single data" 313 here refers to the presence of just one single, isolated data point within the column) shows 314 that, overall 14.7% of all streaks exceed 0 dBz in the lowest 0.4 km (white box in Figure 315 S4b). Furthermore nearly all points within this region originated from higher layers and 316 follow a trajectory of increasing reflectivity with decreasing height (negative inclination). 317 Similarly 20.8% of all streaks reach low reflectivities of  $-25 \, \text{dBZ}$  below  $1.2 \, \text{km}$ . This time a 318 positive inclination can be observed backtracking these points where reflectivities increase 319 with altitude. Thus, in this case, the CFAD provides a mean representation of the aggregated 320 vertical evolution of precipitation. 321

We hypothesize that the negative inclination (0 to 20 dBZ; < 1.2 km) in Figure 2e refers 322 to the melting of solid hydrometeors, enhanced melting of graupel, growth of raindrops by 323 selfcollection (collision-coalescence), and larger ice hydrometeors coated with the layer of 324 liquid water. However, the melting of small ice crystals doesn't cause significant changes in 325 radar reflectivity and thus cannot contribute to the negative inclination in the CFAD. Pro-326 cesses involving the growth of graupel particles (riming, deposition, and collisional growth) 327 are unlikely to contribute to the downward slope as virtually no solid surface precipitation 328 was observed during CAPRICORN. 329

Between the positive and negative inclined slopes, the in-cloud layer hydrometeors 330 are visible along a zero-slope bridge structure (-20 to 10 dBZ between 1.2 and 1.6 km). 331 The continuous cloud-precipitation events that pass through the bins within  $-35 \,\mathrm{dBZ}$  to -332 25 dBZ, and 0.4 km to 1.2 km, account for 17.3% of the total timestamps (Figures S4e,f). 333 Furthermore, most of these events begin above 1.2 km and disappear before reaching 0.4 km. 334 This is in good agreement with the physical hypothesis presented for the positive inclination, 335 which is likely driven by the partial evaporation or sublimation of sedimenting rain or ice. 336 Fall streaks disappearing between 1.2 km and 0.4 km then correspond to precipitation events 337 which fully sublimated or evaporated before reaching the surface. 338

This arc structure which characterizes the dominant evolution of precipitation observed during CAPRICORN is well pronounced in the control simulation (Figure 2f). However, the link (from -5 to 0 dBZ; 1.2 to 1.6 km altitude) between the bridge (here, simulated bridge refers the bright band from -25 to 0 dBZ; 1.6 to 2 km altitude) and the downward slope band is poorly represented. This bias is likely caused by the absence of a melting scheme within PAMTRA and the low vertical resolution of the model output. From the negative inclination of the arc (reflectivity band between 0 and 20 dBZ), the cloud-precipitation

streaks from the bridge firmly reduce to 24%, 11% and 9% below  $1.2 \,\mathrm{km}$  towards near-346 surface, whereas 25%, 24% and 26% were observed during CAPRICORN. The decreasing 347 percentage is either related to a steady decline in raindrop size due to evaporation if the 348 downward change in reflectivity of the streaks is negative, or an increase in raindrop size 349 due to collision-coalescence if the downward change in reflectivity is positive. Meanwhile, 350 percentage increases are associated with an abrupt loss in raindrop size as the reflectivity 351 streaks pass through the multiple reflectivity bins inside the height bins less than 0.4 km. 352 This may result in larger raindrops in the control simulation as their evaporation is more 353 effective at altitudes below 0.4 km in CAPRICORN. To better understand the origin of the 354 bridge structure, the contribution of each hydrometeor species was analyzed individually. 355 This was done to get a sense of the relative importance between the individual hydrometeor 356 species. However, one cannot expect the individual contributions listed in Table S1 to 357 be additive. We find that graupel hydrometeors alone contribute 66% to the total bridge 358 reflectivity structure in the control simulation. Thus in ICON, precipitation statistics are 359 largely influenced by the in-cloud formation and sub-cloud layer evolution of graupel. 360

Here, we compare the simulated statistics and variability of precipitation between obser-361 vations and simulations across a single track observed from the ship over a two-day period. 362 Thus, it is unlikely that these single track measurements capture the entire variability of 363 the low cloud-precipitation system. To account for that, we generate a small ensemble of 364 theoretical tracks in the simulations to compare against the observations. In addition to the 365 ship route, 10 additional tracks are constructed with a 0.2 degree offset (Figure S5). This 366 yields a total of 11 tracks across which the simulated statistics from point measurements are 367 compared with the observations. The normalized CFAD considering the full track ensemble 368 (Figure S6) for the control simulation qualitatively agrees with its same simulation (Figure 2f) just one versus 11 tracks. An average decline in mean bridge reflectivity over all tracks of 370 10.2% was simulated. This indicates that the single-track observations over this time period 371 are sufficiently long to characterize the variability of spatio-temporal intermittent vertical 372 precipitation structures. 373

Figure 2d shows that the simulated cloud phase (see section 2.3 for the definition) 374 along the ship track qualitatively agrees with the phase distinction of the merged radar-375 lidar product (Figure 2c). Furthermore, the simulated MPCs are enriched with graupel. It 376 is evident that all of the graupel particles (hatching in Figure 2d) melt near the melting level. 377 378 In general, radar reflectivity increases towards the ocean surface by collision-coalescence that efficiently occurs on larger raindrops. The larger raindrops are more likely to occur either due 379 to the high ambient relative humidity at low levels that reduces the homogenization of the 380 rain drop size spectrum through evaporation. Additionally, weaker updrafts in comparison 381 with the raindrop fall velocity (weaker convection) can contribute to this effect as the vertical 382 segregation by rain drop sedimentation speed is amplified. Most of the simulated surface 383 precipitation timestamps in the ship track exhibit this phenomenon along the reflectivity 384 streaks. Additionally, the mean Doppler velocity (MDV) also shows the growth in raindrop 385 size driven by collision-coalescence (Figure S3b). For example, the precipitation rate of 386  $5.6 \,\mathrm{mm}\,\mathrm{h}^{-1}$  immediately after the 24<sup>th</sup> hour (Figure 3b) has an increase in reflectivity of 387 >20 dBZ (Figure 2b) near the ocean surface. Similarly, the MDV decreases to  $-3.5 \text{ m s}^{-1}$ 388 below the melting level but slightly increases to  $-3.3 \,\mathrm{m \, s^{-1}}$  below 0.4 km. This may be due to 389 the partial evaporation of the raindrops near the ocean surface. The subcloud evaporative 390 cooling from precipitation reduces the near-surface air temperature and increases the relative 391 humidity. The decrease in near-surface air temperature is connected with the emergence of a 392 surface cold pool, which is a significant criterion for boundary layer decoupling. Further, this 393 increases the surface SHF and decreases the surface LHF. Increased SHF and decreased LHF 394 are driven by the increase in the difference between the near-surface air temperature and SST 395 for the former and increased RH for the latter. These processes were well observed during 396 CAPRICORN (Lang et al., 2021), and across many timestamps in the control simulation 397 (Figure 3a). 398



Figure 2: Time-height cross-section with 1-min temporal resolution of (a) BASTA radar reflectivity, (b) simulated radar reflectivity, (c) observed radar-lidar merged cloud-precipitation phase and (d) simulated cloud-precipitation phase. Isotherms in °C (black lines). Normalized contoured frequency by altitude diagrams (CFAD) with 1-min resolution for the case study period of (e) observed radar reflectivity and (f) simulated reflectivity. Simulated data corresponds to control simulation. Case study period:  $26^{\rm th}$  of March 2016 at 00:00:00 UTC to  $28^{\rm th}$  of March 2016 at 00:00:00 UTC. IV, ice virga; MP, mixed-phase; LW, warm liquid water.

Among the total cloud-precipitation occurrence fraction of 71.1% along the ship track 399 for 1M.90ND, 3.6% occurs within the first 6 hours (succeeded by closed to open cells transi-400 tion or advection) and 24.8% occurs in the final 12 hours of the simulation period. Similarly, 401 among the total cloud-precipitation occurrence fraction of 52.4% observed during CAPRI-402 CORN, 6.4% occurs within the first 6 hours and 19.5% occurs in the final 12 hours of the 403 simulation period. This negative bias in the initial period and the positive bias in the final 404 period for the cloud-precipitation occurrence fraction may be the result of the SST bias 405 correction. A positively biased SST can cause excessive deepening of the boundary layer 406 by overestimating the entrainment of free tropospheric dry air, which can cause the under-407 estimation of the low-cloud fraction (Bretherton & Wyant, 1997; Sandu & Stevens, 2011; 408 Lang et al., 2021). The initialized SST is positively biased during the first 6 hours of the 409 simulation period and negatively biased during the final 12 hours (Figure S1a), explaining 410 why the simulated occurrence fraction or cloud development was lower for the former and 411 higher for the latter. 412

Figure 3b shows that low precipitation rates are observed during CAPRICORN and 413 1M.90ND until the onset of open-cell MCC (open-cell period: 06 to 42 hours). Further-414 more, the total accumulated precipitation is realistic at the end of the two days (Figure 415 3c). Precipitation hardly occurs in the control simulation until 19 hours, whereas frequent 416 precipitation events are observed during this period in the open-cell region. The mean  $(95^{\text{th}})$ 417 percentile) precipitation rate of CAPRICORN and the control simulation are  $0.046 \,\mathrm{mm}\,\mathrm{h}^{-1}$ 418  $(0.05 \,\mathrm{mm}\,\mathrm{h}^{-1})$  and  $0.051 \,\mathrm{mm}\,\mathrm{h}^{-1}$   $(0.13 \,\mathrm{mm}\,\mathrm{h}^{-1})$  respectively. In addition, the occurrence of 419 only few of these events can drastically alter the accumulated precipitation as seen after 420 20 and 24 hours. Although the timing of 1M.90ND precipitation rates doesn't agree well 421 with the observations along the ship track, the interquartile range of quasi-ensemble accu-422 mulated precipitation shows an outstanding agreement with the observations (Figure 6b). 423 The control simulation is skewed to the right (Figure S7), which shows that the stronger 424 precipitation events  $(>1 \text{ mm h}^{-1})$  are sparsely distributed with a mean frequency of occur-425 rence of 3.17 as compared to CAPRICORN with 3.67. Furthermore, the variability of the 426 accumulated precipitation increases considerably in the southeast of the CAPRICORN 427 track, while it differs modestly for most of the tracks in the northwest region (Figure S7 428 and Table S2). 429

The time series of surface precipitation is well aligned with the radar reflectivity pro-430 files in both observation and 1M.90ND. Thus we can combine both measurements to learn 431 more about near-surface precipitation characteristics. By correlating the radar reflectivities 432 at 75 m altitude (where ground BASTA radar first detected the signal) and the observed 433 surface precipitation, the minimum reflectivity associated with at least  $1 \text{ mm h}^{-1}$  of surface 434 precipitation is 1 dBZ. However, 52.6% of surface precipitation rates lower than 1 mm h<sup>-1</sup> 435 are associated with reflectivities larger than 1 dBZ. Using the PAMTRA reflectivities for 436 1M.90ND and the surface precipitation rates,  $1 \text{ mm h}^{-1}$  are associated with a considerably 437 larger minimum reflectivity of 10.8 dBZ. However, only 38.2% of lower precipitation rates 438 are associated with higher reflectivities. Similarly, for precipitation rates of at least  $1 \text{ mm h}^{-1}$ 439 to occur, a maximum criteria of  $-1.96 \,\mathrm{m\,s^{-1}}$  (-2.86  $\mathrm{m\,s^{-1}}$ ) MDV is identified for CAPRICORN 440 (1M.90ND). Yet, 71.4% (24.5%) of lower precipitation rates fall below this criteria. As a 441 result, the minimum reflectivity (maximum MDV) criteria during the occurrence of sur-442 face precipitation above  $1 \text{ mm h}^{-1}$  with respect to minimum reflectivity (maximum MDV) 443 is positively (negatively) biased for the control simulation. Furthermore, the number of 444 events having precipitation rates below 1 mm h<sup>-1</sup> with respect to the minimum reflectivity 445 and maximum MDV is negatively biased for the control simulation (Figure S3b). Since 446 reflectivity is proportional to the sixth power of the size of hydrometeors of similar phase 447 and MDV decreases with an increase in the size of hydrometeors, this reveals that the con-448 trol simulation generates larger near-surface raindrops. This explains why the near-surface 449 relative occurrence frequency over 10 dBZ in the simulation is higher than observed (Figures 450 2e and 2f). However, it is important to keep in mind that the Doppler radar was not on a 451



Figure 3: Time series of (a) LHF, SHF, temperature, and relative humidity for simulation, (b) simulated and observed surface precipitation rate (mm h<sup>-1</sup>). (c) Histograms of precipitation rate for CAPRICORN (black) and simulation (green) along ship track. LHF, latent heat flux. SHF, sensible heat flux. The simulated data corresponds to the control simulation with a 1-min temporal resolution. Simulation period:  $26^{\text{th}}$  of March 2016 at 00:00:00 UTC to  $28^{\text{th}}$  of March 2016 at 00:00:00 UTC. Prec., precipitation rate; Acc. Prec., accumulated precipitation.

452 stable platform, which means that the observed MDV may be subject to greater uncertainty.

Although the reflectivity plots and CFADs provide insight into the microphysics of 453 clouds and precipitation of the sampled SO stratocumuli, a statistical analysis of reflectivity 454 that describes the intensity and duration of cloud-precipitation events can help us under-455 stand them better. Figures 4a to 4d show the fraction of cloud-precipitation events along the 456 ship track categorized based on reflectivity between -20 and 20 dBZ incremented by a step 457 of 10 dBZ. The fraction is calculated as the ratio of the duration of events in a reflectivity 458 range to the total duration of cloud-precipitation events along the entire ship track. While 459 lines and shading characterize the average intensity and duration of events, the distribution 460 of individual dots (Figure 4e to 4h) characterizes the variability of those cloud-precipitation 461 events. The observed lower reflectivity events (Figures 4a and 4b) dominate the cloud layer, 462



Figure 4: The cloud-precipitation occurrence (event) fraction (also termed as cloud cover) with height is categorized into reflectivity from (a) -20 to -10 dBZ, (b) -10 to 0 dBZ, (c) 0 to 10 dBZ and (d) 10 to 20 dBZ. The scatter plot represents the length of continuous cloud events with height, in the reflectivity range of (e) -20 to -10 dBZ, (f) -10 to 0 dBZ, (g) 0 to 10 dBZ and (h) 10 to 20 dBZ, where the lines represent the mean length of continuous cloud events in minutes (scatter mean). The scatter points (which are shown for control simulation only) become darker as the overlay of the data increases. The green shading corresponds to the quasi-ensemble variability (interquartile range) for the control simulation. This analysis takes into account the data throughout the ship track for the entire case period. The legends in 4d are common for all the subfigures.

as smaller hydrometeors (both liquid and ice) are captured in these reflectivity ranges.
In a subsaturated environment, the smaller raindrops (ice crystals) evaporate (sublimate)
efficiently since the surface-to-mass ratio is higher when compared with the larger raindrops
(ice crystals). Since larger raindrops have higher reflectivities than solid hydrometeors
(where both of them are equal in size), they are recorded in the highest reflectivity range
(Figure 4d).

Similar distinct intermittent cloud events are simulated in 1M.90ND as were observed 469 by the BASTA radar. However, the frequency of cloud events (Figure 4a and 4b) and their 470 continuous duration (Figures 4e,4f) between -20 and 0 dBZ are overestimated above the 471 melting level (approximately 1.2 km in altitude). The figures show that larger raindrops and 472 graupel (between 0 and  $10 \, \text{dBZ}$ ) persist on far more successive timestamps than observed 473 (Figure 4g), but are sparsely distributed (Figure 4c). Table S1 summarizes the range of 474 simulated reflectivities for each hydrometeor. The simulated radar reflectivities  $>10 \,\mathrm{dBZ}$ 475 are solely due to larger raindrops. In this reflectivity range, the number of events that occur 476 along the ship track is underestimated by 26% below 0.8 km altitude, although their mean 477 event length is 3 times longer (Figures 4d and 4h). 478

#### 479 **3.2** Microphysical Sensitivities

We performed bulk microphysics sensitivity experiments to investigate the shortcomings of the control simulation (1M.90ND) with respect to the cloud microphysical processes, cloud occurrence, and surface precipitation. The reflectivity cross-section of the control simulation generates homogeneous clouds with constant CTHs after 36 hours of simulation time that

were not observed (Figures 2a and 2b). This observed variability in CTH from 36 hours 484 onward is qualitatively better captured in all 2M simulations (Figure 2a and Figure S8). The 485 1M simulation with reduced CDNC to  $20 \,\mathrm{cm}^{-3}$  qualitatively agrees with the arc structure of 486 the observed CFAD (Figure 5a), however the bridge reflectivity (sum of reflectivity samples 487 between -25 to 0 dBZ; 1.6 to 2 km altitude) reduces by 5% (Table S1c), and the bridge shifts 488 to the left. The reduced CDNC experiment results in a decline in cloud water reflectivity 489 and an increase in raindrop reflectivity in the CFAD bridge (Table S1). This is due to an 490 inverse Twomey effect where the reduced CDNC leads to larger cloud droplets and more 491 effective autoconversion. Meanwhile, it has also reduced the graupel reflectivity by 5.1%. 492 Surprisingly, all the state-of-the-art 2M microphysics sensitivity experiments fail to achieve 493

dBZ	Statistics	CAP	1M.20ND	$\begin{array}{c} 1\mathrm{M.90ND} \\ \mathrm{(ctrl)} \end{array}$	2M.P	2M.HM	2M.HM.BR03
10 +- 20	$\mathbf{EF}$	0.36	0.60	0.60	0.41	0.37	0.38
-40 to 20	MEL	9.10	45.41	41.33	21.25	22.0	22.92
20 + - 10	EF	0.11	0.26	0.24	0.11	0.10	0.10
-20 to -10	MEL	2.42	8.3	8.15	3.25	3.49	3.93
10 to 0	EF	0.13	0.18	0.21	0.11	0.11	0.12
-10 to 0	MEL	2.77	9.30	10.67	5.98	7.21	6.32
0 to 10	EF	0.08	0.03	0.05	0.08	0.08	0.07
	MEL	2.0	3.0	2.0	3.29	4.5	6.88
10 to 20	$\mathbf{EF}$	0.03	0.02	0.02	0.02	< 0.01	0.01
	MEL	1.0	3.0	5.0	1.0	1.0	3.0

Table 2: Reflectivity statistics derived from Figure 4. 'EF' is the event fraction of the simulations and CAPRICORN at the altitude where their maximum event fraction occurs. 'MEL' is the mean event length (min) of the simulations and CAPRICORN at the altitude where the maximum event fraction of the respective simulation and CAPRICORN occurs. CAP, CAPRICORN. ctrl, control simulation.

the CFAD reflectivity arc, which is a proxy for cloud-precipitation vertical structure. The 494 mean contribution of the graupel bridge reflectivity is reduced by 80% for 2M microphysics 495 experiments and the mean increase in graupel for the experiments with secondary ice pro-496 cesses is just 23% with respect to 2M.P. Irrespective of the increase in rain and snow re-497 flectivities in all 2M simulations, the reflectivity of the bridge is reduced by 46% (49%) 498 with respect to the control simulation (BASTA radar). This demonstrates the importance 499 of graupel processes in the SO mixed-phase Sc clouds sampled during CAPRICORN. The 500 variations in hydrometeors other than graupel in the bridge are also noticeable, although 501 the largest value of total graupel reflectivity due to its size and number concentration makes 502 it dominant in the cloud layer (Table S1b). Meanwhile, the 2M.HM simulation generates 503 very small cloud particles as their maximum reflectivity is 2.6 times less than the control 504 simulation (Figure 2f and 5c). 505

In Table 2, the mean event (cloud-precipitation) length and the occurrence fraction have 506 been derived for all experiments at the altitude of their maximum mean event fraction. All 507 simulated values are overestimated. However, the 2M experiments show a better agreement 508 with the observations than the 1M simulations. For all simulations, this agreement does not 509 hold true across all altitudes. This shows that the microphysics of ICON simulations (1M 510 and 2M) do not perfectly replicate the observed cloud vertical structure along the ship track. 511 Figure 6 shows the simulated and observed surface precipitation along the ship track for the 512 entire case period. All simulations except 2M.HM.BR03 show intense precipitation, hence 513 the change in the accumulated precipitation in 2M.HM.BR03 is gradual at all timestamps. 514 As expected, none of the experiments replicate the timing of the precipitation rate, the pro-515 file and variability of accumulated precipitation as compared to the observation. Although 516 all the single track simulated data (except 2M.HM.BR03) overestimate the accumulated 517



Figure 5: Contoured frequency by altitude diagrams (CFAD) with 1-min temporal resolution for the entire case study period of a) 1M.20ND, (b) 2M.P (c) 2M.HM and (d) 2M.HM.BR03. CFAD is normalized with the total samples in every reflectivity bin. The numerical data at the top of CFAD are the ratios of cumulated samples in every reflectivity bin to the highest cumulated samples from all the reflectivity bins. Case study period:  $26^{\text{th}}$  of March 2016 at 00:00:00 UTC to  $28^{\text{th}}$  of March 2016 at 00:00:00 UTC.

precipitation along the ship track at the end of two days, the ensemble accumulated precipi-518 tation variability (interquartile range) for 1M.90ND (the full variability is available only for 519 1M.90ND due to output limitation) increases with time, and further overlaps with that of 520 other experiments (in particular during a large time period on  $27^{\text{th}}$  of March 2016). While 521 the observations are entirely within the spatio-temporal variability of 1M.90Nd, a maximum 522 of 66% for 2M.P and a minimum of 21% for 2M.HM.BR03 overlap with the variability of 523 1M.90ND. This suggests that due to the small sample size (two-day) and wide confidence 524 interval (provided the ensemble variability within each experiment is significant), it remains 525 difficult to characterize the full spatio-temporal variability of the surface precipitation. 526

The simulated domain mean surface precipitation (domain mean CB precipitation 527 rates) are  $0.045 \text{ mm hr}^{-1}$  (3.6 mm hr $^{-1}$ ) for 2M.P,  $0.053 \text{ mm hr}^{-1}$  (3.3 mm hr $^{-1}$ ) for 2M.HM, 528 and  $0.061 \,\mathrm{mm \, hr^{-1}}$  (2.7 mm hr<sup>-1</sup>) for 2M.HM.BR03. This shows that despite a mean in-529 crease in total ice number concentration by two (three) orders of magnitude for 2M.HM 530 (2M.HM.BR03) compared with 2M.P (Figure S9), the mean surface precipitation rate only 531 modestly increases, and the CB precipitation rate even decreases. This result is somewhat 532 counter-intuitive as one would expect increased cloud glaciation due to increased ICNC and 533 thus increased growth rates by deposition (e.g. Vergara-Temprado et al. (2018)). Yet, CB 534 precipitation rates decrease in our simulations. We cannot uniquely identify what is causing 535 this decrease by 6% in 2M.HM and 23% in 2M.HM.BR03 with respect to 2M.P. However, 536 the following processes may play a role. Firstly, the rate of ice hydrometeor growth through 537 riming with cloud droplets is decreased in 2M.HM.BR03 which further reduces CB precipi-538



Figure 6: Time series of simulated and observed (a) precipitation rate (mm h<sup>-1</sup>) and (b) accumulated precipitation (mm). Simulated data corresponds to control simulation and all the simulations in the bulk microphysical sensitivity analysis. The green shading corresponds to the quasi-ensemble variability ( $25^{\text{th}}$  and  $75^{\text{th}}$  percentiles) of accumulated precipitation for the control simulation.



Figure 7: The relative percentage contribution of various cloud types (liquid - blue, mixed - green and ice - red) to surface precipitation along the ship track is stacked on top of one another. Data is analyzed for the entire case study period ( $26^{\rm th}$  of March 2016 at 00:00:00 UTC to  $28^{\rm th}$  of March 2016 at 00:00:00 UTC).

tation (Figure S10). Secondly, the very small ejected ice crystals during collisional breakup
may not be favorable for the formation of snow (ice-ice aggregation) and growth of snow
(ice-snow collision). Thirdly, unlike HM, collisional breakup reduces the size and eventually
the mass of individual solid hydrometeors by ice fragmentation, thus reducing their terminal fall velocity. Fourthly, while depositional growth increases, it does not compensate for

the decrease in size by fragmentation. Thus terminal fall velocity remains low. It is likely that combined effect of: reduced terminal fall speed of ice crystals, and decreased riming efficiencies, reduce the mean CB precipitation rate in 2M.HM.BR03 as compared to 2M.HM.

Figure 7 shows the simulated cloud type contribution to surface precipitation rates. 547 Here, the cloud types are categorized as liquid (liquid CB with liquid CB precipitation), ice 548 (ice CB with ice CB precipitation), and mixed (CB and CB precipitation having different 549 phases). The Twomey effect is illustrated clearly by the drop of 29% in liquid cloud con-550 tribution to precipitation rates between 1M.20ND and 1M.90ND. The ice (mixed) clouds 551 contribute 67% (33%) to the observed precipitation rates, and the impact of ice (mixed) 552 clouds on all the simulations is lower (higher). Ice and mixed-phase clouds account for 553 an increase of 32% in surface precipitation rates from 2M.P to 2M.HM, but this fraction 554 decreases by 6% from 2M.HM to 2M.HM.BR03. The fractional decline could be explained 555 by the fact that (i) smaller ice particles require less latent heat to melt, as they cross the 556 melting line within the cloud layer and (ii) reduced ice mass sedimentation as stated in the 557 previous paragraph. 558

#### 559 3.3 Impacts on Radiation

Figure 8a shows the observed and simulated surface downwelling SW radiation (SW<sub>surf.down</sub>), 560 as well as the liquid, mixed, and ice CT fractions. In general, we find that the lower the com-561 bined liquid and mixed CT fraction, the higher the mean SW<sub>surf.down</sub> is in all the simulations. 562 This is entirely consistent with the larger scattering efficiency of the far more numerous and 563 smaller cloud droplets as compared the few and large ice crystals (Greenwald et al., 1995). 564 We further observe that changes in cloud phase area fraction have a considerably larger 565 impact on SW<sub>surf.down</sub> than microphysical effects such as Twomey. An increase in ice-phase 566 fraction in 2M.HM.BR03 with respect to 2M.HM increases  $SW_{surf,down}$  by  $8 W m^{-2}$ . This 567 is twice as large as the decrease through the Twomey effect by  $4 \,\mathrm{W\,m^{-2}}$  between 1M.20ND 568 and 1M.90ND. Hence, these two simulations (2M.HM and 2M.HM.BR03) generate optically 569 thicker clouds. In all other simulations the underestimation in  $SW_{surf,down}$  is likely caused 570 by both: an overabundance of liquid-containing clouds and overestimated optical depth. 571

As discussed above, CTP plays a predominant role in constraining the cloud-top radia-572 tive effect. The histograms of relative occurrences of CTP binned into  $5^{\circ}C$  CTT are shown 573 in Figure 8b. The sampled open-cell (36 hours from 26<sup>th</sup> of March 2016 at 06:00:00 UTC) 574 CTP from HIMAWARI along the ship track is classified with 78.3% as liquid. The total liq-575 uid fraction consists of 49.8% warm liquid water (LW) and 28.5% SLW. Meanwhile, merely 576 5.9% of all clouds in the control simulation are classified as liquid at CT with 1.1% LW and 577 4.8% SLW. The narrowly distributed simulated CTT with the mode between  $-10^{\circ}$ C and 578 -5°C holds 75.6% mixed-phase CTs against the observed 3.1%. Further, HIMAWARI clas-579 sifies only 8.5% as mixed-phase open-cell stratocumuli at CT along the ship track, whereas 580 87.78% are identified as such in the control simulation. This may be due to the lower vertical 581 resolution, inadequate representation of CT turbulence, dissipation of the sharp tempera-582 ture inversion due to TKE centered around the CT instead of being at or below the CT, 583 poor updraft velocity to push cloud droplets to the CT (Vignon et al., 2021), and possibly overprediction of ICNC by the temperature-dependent Cooper parameterization for ice nucleation (Cooper, 1986). No open-cell Sc CTTs are simulated (1M.90ND) below -15°C and 586 above  $5^{\circ}$ C, whereas 13.1% (ice) and 21.8% (LW) CTs were observed below and above these 587 limits along the ship track. However, the warm clouds in HIMAWARI may be subject to 588 large uncertainties since the surface temperature and emissivity influence the CTT retrievals 589 (Huang et al., 2019). Overall, the control simulation along the ship track (open-cell period) 590 overestimates the liquid and mixed-phase CTs by 35.2%, and overestimates the cloud oc-591 currence by 26.1%, resulting in the underestimation of surface downwelling SW radiation 592 by 42.7%, compared to the observations. 593



Figure 8: HIMAWARI and simulated data along the ship track during the open-cell period. (a) Surface downwelling shortwave radiation (W m<sup>-2</sup>) and the total CT fractions with relative contributions of liquid (blue), mixed (green), and ice (red) phase (stacked one over the other). (b) Histograms of CTP fractions as a function of the cloud-top temperature (CTT) with the bins of 5°C. CT, cloud-top. HIMAWARI data is obtained from Huang et al. (2019); Lang et al. (2021).

Although the CTP distinguished with CTT doesn't vary substantially for the reduced 594 CCN experiment (1M.20ND), the occurrence of SLW significantly increases in the 2M ex-595 periments between  $-10^{\circ}$ C and  $-5^{\circ}$ C (Figure 8b). Since many cloud event streaks are entirely 596 liquid with no traces of solid hydrometeors (Figure S11), they increase the CT SLW frac-597 tion. As opposed to the Cooper ICNC curve, the observationally constrained INP immersion 598 freezing parameterization with considerably lower INP background concentrations has pro-599 duced MPCs only at a few instances along the ship track. Although, the in-cloud domain 600 mean IWP has increased to  $50 \,\mathrm{g \, m^{-2}}$  in the 2M.P simulation (Figure S9). This shows that 601 the immersion INP parameterization adjusted for the SO remote region is insufficient to 602 reduce cloud-radiative biases caused by inaccurate representations of cloud phase and the 603 partitioning of the total water path between LWP and IWP. Similar to the control simula-604 tion, all the sensitivity experiments cluster 80% of the simulated CTs between  $-10^{\circ}$ C and 605 -5°C. Warm CTs above 5°C are still missing. However, the increase in the ice occurrence 606 fraction at CT is consistent with the activation of secondary ice processes between -10°C 607 and  $-5^{\circ}C$  (2M.HM and 2M.HM.BR03). 608

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### 3.4 Perturbed-Parameter Experiments to enhance graupel formation in 2M simulations

As discussed in section 3.2, the state-of-the-art 2M microphysics scheme in ICON dis-611 plays stronger biases in the vertical structure of precipitation than the 1M simulations. Here, 612 we look at the microphysical pathways to understand the role of individual processes for 613 both schemes in detail (Figure 9). As discussed earlier, graupel particles play a significant 614 role in the occurrence of the bridge in the cloud layer in CFAD diagrams. The time-height 615 cross-section of the simulated phase shows that graupel (hatching in figures) covers a larger 616 sample in 1M (Figure 2d and Figure S11a) than in all the 2M simulations (Figures S11b to 617 S11d) above the melting level. The 1M and 2M microphysical pathway analysis discussed in 618 this section is obtained from the 1M.90ND and 2M.HM simulations on 27<sup>th</sup> of March 2016. 619 Among the graupel growth processes shown in Figure S12 and Figure 9, CG2G\_rim (cloud-620 graupel to graupel riming) and RG2G\_rim (rain-graupel to graupel riming) are the dominant 621 processes. The CG2G\_rim process rate is higher in the cloud layer in the 1M scheme (9.13) 622 than in the 2M scheme (2.30). Note that all process rates are normalized for comparability 623 by WVL as described in section 2.3 and are thus unitless. Although RG2G\_rim is not 624



Figure 9: Flowchart of the microphysical processes on 27<sup>th</sup> of March 2016 for (a) 1M.90ND, (b) 2M.HM. The ratios of each microphysical process rate to the rate of total water vapor loss (WVL) are shown within parenthesis (refer to equations 1 and 2). The abbreviations are as follows: C, cloud ice. I, cloud ice. R, Rain. S, snow. G, graupel. H, hail. V, vapor. au, autoconversion. ac, accretion. frz, freezing. melt, melting. shed, shedding. evp, evaporation. cond, condensation. sub, sublimation. dep, deposition. rim, riming. rims, rime splintering. coll, solid hydrometeor collision. agg, aggregation. nuc, ice nucleation.

parameterized in the 1M scheme, the cloud phase time series indicates larger traces of 625 raindrops in the cloud layer in 2M scheme (Figures S11b-d) than in 1M scheme (Figure 2d 626 and Figure S11a). This might be because CG2G\_rim in the 1M scheme is more efficient in 627 scavenging cloud droplets before they grow into raindrops than the CG\_rim and RG\_rim rates 628 in 2M scheme. All graupel formation processes (such as cloud-snow to graupel, ice-rain to 629 graupel, rain-snow to graupel, rain to graupel freezing, and ice to graupel by aggregation) 630 are associated with a lower mass transfer to the graupel category than graupel growth 631 processes (i.e. CG2G\_rim and R2G2G\_rim). Figures 5b to 5d show strong near-surface high 632 reflectivity bands (-20 dBZ to 15 dBZ) with the higher relative frequency of occurrences in 633 the 2M simulations. However, this was not observed during CAPRICORN and not simulated 634 in the 1M scheme. Possible reasons could be a higher (lower) graupel melting rate of 9.70 635 (8.15), a lower (higher) raindrop evaporation rate of 0.57 (1.95), and lower (higher) grauped 636 sublimation rate of 0.14 (0.93) for 2M.HM (1M.90ND) (Figure 9). 637

As a result, raindrop selfcollection may be effective in 2M.HM, which enhances droplet 638 diameter and further increases cloud reflectivity. Among the microphysical processes shown 639 in the flow chart of microphysical pathways, graupel melting is the major source of rain 640 in both schemes for SO Sc clouds. Graupel melting accounts for about 80% of the rain in 641 the 1M scheme and 91% of the rain in the 2M scheme. Furthermore, 24% and 6% of the 642 melted graupel evaporate in 1M and 2M microphysics schemes respectively. Although the 643 new rain particle formation in the cloud layer by autoconversion is larger by a factor of 6 in 644 the 2M scheme, their growth by accretion is reduced by a factor of 2. Hence, the raindrops 645 in the cloud layer might not be large enough to get rimed by graupel. Most raindrops 646 are scavenged in the riming processes in 1M simulations, making it difficult to verify this 647 hypothesis with the existing set of simulations. Thus, we performed further sensitivity 648 experiments (summarized in Table 1) altering parameters affecting graupel generation and 649 growth, either directly, or indirectly to further understand the deficiencies of the simulated 650 vertical structure of precipitation in the 2M simulations. 651

Expt No.	Description	CG2G	G2R	RG2G	G	G
		$_{\rm rim}$	_melt	_rim	_dep	_budget
1	2M.HM * E10	24.80	-108.06	77.52	5.41	9.00
2	2M.P	-14.37	-16.46	-12.09	-31.41	-19.47
3	2M.HM.BR03	5.12	6.75	5.28	1.35	6.08
4	CCN10	-1.09	-8.57	-9.60	-11.59	-7.54
5	CCN1000	-39.71	-45.93	-49.67	-34.84	-41.79
6	aukcc*0.5	2.32	3.88	4.37	0.88	0.72
7	aukcc*2	-1.23	-5.95	-6.91	-1.24	-0.55
8	ice_vel_coef	3.85	-4.04	-5.63	-2.83	-0.32
9	$rain_{atlas}$	-6.90	-4.87	-3.59	-3.96	-6.25
10	$agg_50$	1.45	0.94	1.10	0.53	0.99
11	$agg_200$	-4.41	-2.17	-2.97	-3.64	-2.61
12	gr_d_m	-7.90	-8.53	-9.65	-7.08	0.96
13	gr_d_h	-16.56	-21.51	-24.15	-2.76	5.61
14	gr_v_h	-3.29	-9.28	-12.13	-38.94	-51.70
15	gr_max_dia	-63.85	-76.84	-81.73	-59.72	-60.49

Table 3: The top row (in kg) shows the sum of the product of hourly process rates and volume of each cell for the reference simulation (2M.HM) on  $27^{\text{th}}$  of March 2016. G\_budget (in kg) for the reference simulation refers to the sum of the product of instantaneous graupel mass density and the volume of each cell. All the other rows are percentage changes with respect to the reference simulation. The intensity of the color scale shows the percentage decrease (increase) in red (blue). The table only shows process budgets that exceed 50% of the G\_budget.

To realistically simulate the graupel processes in the SO Sc clouds, it is crucial to 652 analyze their sensitivity to the parameters related to CCN and ice-phase processes. Our 653 small parameter ensemble is motivated by the importance of CG2G\_rim and RG2G\_rim for 654 graupel growth. CCN concentrations are perturbed for the former, and the rain terminal 655 velocity relation (power-law (Seifert & Beheng, 2006), and atlas-law (Seifert et al., 2014)), 656 as a function of its mass, is perturbed for the latter. As reported in Seifert and Beheng 657 (2006), the velocity coefficients of ice crystals are based on the measurements from Locatelli 658 and Hobbs (1974); Heymsfield and Kajikawa (1987). Furthermore, the graupel density and 659 its velocity measured during the winter months of 1971-1972 and 1972-1973 in the Cascade 660 Mountains of Washington (Locatelli & Hobbs, 1974) are used to study the sensitivity of the 661 G\_budget. 662

The 2M.HM simulation (Table 3) is considered a reference experiment in this section. 663 The numbers, except for the G<sub>-</sub>budget in the reference experiment, are averaged hourly and 664 summed over a time period of 24 hours on 27<sup>th</sup> of March, 2016. The G<sub>-</sub>budget in the last 665 column of this experiment refers to the time-space integrated sum of instantaneous hourly 666 graupel mass mixing ratios for the same 24 hours period. All the other rows in this table 667 represent the percentage change with respect to the reference simulation. The increase in 668 CCN from 10 cm<sup>-3</sup> to 1000 cm<sup>-3</sup> results in a monotonic increase in smaller cloud droplets 669 (Twomey & Warner, 1967). This reduces the cloud droplet autoconversion and accretion 670 rates, and further delays the rain to graupel riming process. The net G\_budget is reduced 671 by 41.79%. Similarly, reducing the CCN (CCN10) below a threshold value also reduces the 672 G\_budget and the related process rates. A reduced autoconversion kernel coefficient by a 673 factor of 2 increased the rate of the cloud-graupel riming process by 2.3%, since the rain 674 particle formation slowed down. This modest increase could be attributed to the lower cloud 675 liquid water path (LWP) in 2M simulations compared to 1M simulations. Any increase in 676 graupel density allows for an increase in its mass and hence a modest gain in the G<sub>-</sub>budget. 677 However, the mass and terminal velocity of the hydrometeors are coupled by a power-law. 678 An increase in graupel density or graupel diameter increases the terminal velocity which 679

reduces its residence time, and hence the G\_budget (experiments 13 and 14 in Table 1). The rime splintering process reduces the gap between the simulated and observed ICNC, and also governs the new graupel particle formation processes (experiment no. 15 in Table 1) in the remote environment of the SO boundary layer. Hence, the secondary ice production processes (HM and collisional breakup) lead to an increase in the net G\_budget.

Overall, it is significant that (i) the CCN number concentration affects the G\_budget through the RG2G\_riming process and (ii) the graupel properties (density, velocity, and size) have a strong effect on the net G\_budget. The 2M microphysics sensitivity experiments for SO Sc clouds show that the net G\_budget is at its maximum when: (i) the graupel density, velocity, and size are low, (ii) the power-law captures the raindrop velocity as a function of its mass, (iii) secondary ice production processes are active, and (iv) CCN values are low.

#### <sup>691</sup> 4 Discussion and Conclusions

We have evaluated the ability of kilometer-scale ICON real-case simulations against 692 the observed cloud and precipitation statistics derived from remote sensing and in-situ mea-693 surements during CAPRICORN. In general, the control simulation captured the observed 694 cloud-precipitation vertical structure due to graupel growth by the riming of cloud droplets. 695 A continuous formation of graupel, its growth in the cloud layer, and subsequent melting 696 are crucial processes for realistically representing the cloud-precipitation vertical structure 697 of SO Sc clouds. Further, a lower CCN concentration and increased density, velocity, and 698 size of graupel particles all enhance low-cloud graupel formation. According to the micro-699 physical pathway analysis, graupel melting is a major source of SO Sc precipitation during 700 CAPRICORN. The duration of continuous cloudy elements containing either cloud droplets, 701 rain, or graupel particles is overestimated in all ICON simulations. This results in an over-702 estimated mean duration of cloudy elements along the entire ship track. Thus, the timing 703 of the simulated cloud-precipitation events doesn't agree with CAPRICORN, which is also 704 evident in the comparison with observed surface precipitation rates. The simulated surface 705 precipitation is sparsely dispersed, whereas the OceanRAIN disdrometer measures densely 706 distributed precipitation rates with relatively sharp spikes. Although the simulated accu-707 mulated precipitation at the end of two days is closer to CAPRICORN, the onset of stronger 708 precipitation in the open-cell region is delayed by 9 hours in the simulation. Although the 709 observations are within the simulated range of variability of the control simulation, longer 710 continuous observations within the same cloud regime would be needed to fully constrain the 711 simulated cloud-precipitation statistics. Despite these shortcomings, the control simulation 712 captured the surface cold pool (drop in near-surface air temperature) in many timestamps 713 that favored the occurrence of the transition layer and the decoupling of the boundary layer. 714

The phase distinction from the merged radar-lidar product, the CFAD of radar reflec-715 tivity, and the HIMAWARI CTP confirm the presence of ice in the cloud. We observed 716 that the bridge reflectivity (reflectivity of a sharp horizontal band in the arc i.e., in the 717 cloud layer) is a reasonable proxy for evaluating the cloud layer hydrometeors. According to 718 the independent hydrometeor reflectivity contribution analysis for all simulations, a relative 719 increase in the graupel mass in the cloud layer reduced the gap between the observed and 720 simulated bridge reflectivities, resulting in a more realistic representation of the arc struc-721 ture. The highest contribution of graupel is 66% (1M.90ND) and 59% (1M.20ND) in 1M 722 simulations that realistically represent the observed cloud vertical structure, while it is less 723 than 20% in 2M simulations. In addition to the occurrence of graupel in the cloud layer, all 724 other processes involving graupel and raindrops, such as partially sublimated frozen parti-725 cles, partially evaporated larger raindrops, melting of graupel, raindrop selfcollection, and 726 solid hydrometeors coated with liquid layer during the collision of ice particles with rain-727 drops are also crucial in describing the observed cloud-precipitation vertical structure. The 728 raindrops in the cloud layer (bridge) dominate the reflectivities rather than the graupel in 729 all 2M simulations. The enhanced raindrop reflectivity in the cloud layer did not increase 730 bridge reflectivity, rather, the bridge reflectivity decreased by 46% compared to the control 731

simulation. Theoretically, graupel (rain) contributed reflectivities could be increased (decreased) if efficient in-cloud graupel growth by riming rain scavenges raindrops. Hence, the
bridge statistics clearly emphasize the significance of graupel in SO Sc clouds.

The presence of graupel, which is one of the necessary conditions in HM (Hallett & 735 Mossop, 1974) and an enhancing parameter due to increased collisional kinetic energy in 736 breakup collisions (Phillips, Yano, & Khain, 2017), increases the secondary ice production. 737 We investigated the sensitivity with respect to secondary ice generating processes (HM and 738 collisional breakup) in Sc clouds during CAPRICORN. The maximum reflectivity of cloud 739 740 droplets in the 2M.HM simulation is 2.6 times lower than the control simulation, indicating that cloud droplet size decreased. The reflectivity event fractions of all the 2M simulations 741 show that the larger raindrops (20 > dBZ > 10) evaporate effectively in the sub-cloud layer 742 and increase the smaller raindrop number concentration in the intermediate reflectivity 743 range (10 > dBZ > 20), and hence the occurrence of strong frequency of occurrence band 744 near the surface in the 2M CFAD diagrams. This indicates that the near-surface raindrops 745 in all 2M simulations are smaller compared to 1M simulations. Although the domain mean 746 total ice number concentration (total ice water path) in 2M.HM.BR03 increase by roughly 747 10 (1.4) times compared to 2M.HM, the domain mean precipitation increases by just 1.2 748 times. Hence, despite the increase in the total ice number concentration through collisional 749 breakup, the precipitation statistics remain dominated by melted graupel containing primary 750 INP along the ship track. 751

The SW<sub>surf,down</sub> along the ship track in the control simulation is negatively biased 752 by 43% due to the overestimation of the liquid and mixed-phase CT by 35%, and the 753 cloud occurrence by 26%. Furthermore, the  $SW_{surf,down}$  of all simulations is negatively 754 biased irrespective of the extent of liquid CT fraction, yet, most of the simulated total 755 liquid and mixed-phase CT fractions are higher than observed during CAPRICORN. The 756 control simulation failed to produce the dominant liquid CTs, instead, 87.78% are mixed-757 phase with just 8.5% diagnosed as such in HIMAWARI retrievals. This could be due to a 758 variety of factors, one of which is the insufficient vertical resolution in all simulations that 759 would be required to fully represent a supercooled liquid layer on top of the mixed-phase 760 cloud. It is worth noting that the 2M simulations (2M.HM and 2M.HM.BR03) adjusted 761 for a remote INP environment over the SO generate optically thicker clouds, as primary 762 nucleation is considerably reduced and indeed many cloud profiles are entirely liquid. All 763 other simulations generate positively biased cloud cover and/or optically thicker clouds. 764 Thus the cloud radiative bias in this particular regime is contrary to the climatological bias 765 (Trenberth & Fasullo, 2010; Bodas-Salcedo et al., 2014; Vergara-Temprado et al., 2018). 766

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### Supporting Information for "An evaluation of kilometer-scale ICON simulations of mixed-phase stratocumuli over the Southern Ocean during CAPRICORN"

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#### 1. PAMTRA for ICON simulations

Passive and Active Microwave TRAnsfer (PAMTRA) is made to accommodate microphysical outputs from both 1M and 2M ICON simulations (Mech et al., 2020). The active radiative transfer part includes the forward simulation of the bottom-up radar reflectivity profiles, and Doppler spectrum and its moments. The 1M scheme that simulates prognostic mass mixing ratio is assumed to have a monodisperse particle size distribution for both cloud droplet and cloud ice hydrometeors. Inverse exponential size distribution is assumed for the other hydrometeor categories. The parameters of four-parameter gamma distribution are set to transform into a monodisperse (all the four parameters = 0) and inverse exponential size distribution (shape parameter = 0 and power factor = 1) (Petty & Huang, 2011; Wu & McFarquhar, 2018; Mech et al., 2020), with the maximum fixed size for the former and size computation according to mass-size power-law relation for the latter. All six hydrometeor categories in 2M are assumed to be distributed according to modified four-parameter gamma distribution, while the sizes are computed from mass using power-law relations. In our PAMTRA offline simulations, cloud droplets, rain, graupel and hail follow mie scattering, whereas ice and snow follow self-similar Rayleigh–Gans scattering.

#### 2. Parameterization for cloud droplet number concentration

In 2M scheme, the cloud droplet number concentration (CDNC) at the cloud base is parameterized using the regression equations with CDNC as a function of condensation nuclei (CN) concentration, width of their size distribution and cloud base velocity (Segal & Khain, 2006). The number of droplets to be added in the cloud is provided by the look-up tables for a prescribed list of number concentrations and mean radii of the CN size distribution, with the interpolated cloud base velocity and the width of CN distribution, making it prognostic in the 2M scheme.

#### 3. Parameterization for ice crystal number concentration

In 2M scheme, the total potential ice nucleating particles (INPs) are determined based on the McCluskey, Ovadnevaite, et al. (2018) for sea spray aerosols (Equation 1) and Demott et al. (2015) for mineral dusts (Equation 2). The immersion freezing occurs in the region where the supersaturation with respect to ice is greater than 100%, the temperature is lower than  $-5^{\circ}$ C, and the cloud droplet mass mixing ratio is higher than 1E-20 kg m<sup>-3</sup>.

$$n_{\rm SSA, INPs}(T) = exp[-0.545(T - 273.15) + 1.0125] * S_{\rm SSA} * 0.001$$
(1)

$$n_{\rm dust\_INPs}(T) = exp[0.46(273.15 - T) - 11.6] * (n_{\rm 500nm})^{1.25}$$
(2)

Here,  $n_{SSA_{INPs}}$  is the potential INP number concentration from the sea spray aerosols (L<sup>-1</sup>);  $n_{dust_{INPs}}$  is the potential INP number concentration from the mineral dust (L<sup>-1</sup>); T is the temperature (K);

 $S_{SSA}$  is the surface area concentration of the sea spray aerosols (m<sup>2</sup> m<sup>-3</sup>). The mean of  $S_{SSA}$  for the two-day period (=22.1829E-6 m<sup>2</sup> m<sup>-3</sup>) is derived from McCluskey, Hill, et al. (2018);  $n_{500nm}$  is the number concentration of mineral dust particles greater than 500 nm in size (cm<sup>-3</sup>). This value is calculated by equating the the total INP ( $n_{SSA\_INPs} + n_{dust\_INPs}$ ) number concentration as 0.0046 L<sup>-1</sup> at -20°C (McCluskey, Hill, et al., 2018) in March-April 2016.





Figure S1: (a) Uncorrected (left-hand side) and corrected (right-hand side) SST contours in the simulation domain on 25<sup>th</sup> of March 2016 at 12:00:00 UTC with the two-day ship track (green). Time series for the entire ship track of (b) SST (°C), (c) SHF (W m<sup>-2</sup>) and (d) LHF (W m<sup>-2</sup>). SST, sea surface temperature; SHF, sensible heat flux; LHF, latent heat flux.



Figure S2: Thermodynamic profiles from upper-air radiosondes (black lines) and control simulation (1M.90ND - green lines) at the same location on (a),(c)  $26^{\text{th}}$  of March 2016 at 01:42:00 UTC and (b),(d)  $26^{\text{th}}$  of March 2016 at 06:24:00 UTC. Dashed lines in green (black) represent the location of simulated (observed) transition layer.  $\theta$  represents potential temperature.

The boundary layer decoupling from the thermodynamic profile is identified by the presence of a transition layer that separates the cloud and subcloud layer. A strong decrease in mixing ratio and an increase in potential temperature characterize the transition layer. The conditional  $\mu$  parameter which is defined as  $\mu = \delta \theta / \delta P - ((0.608 \theta / (1+0.608r)) \delta r / \delta P)$  can identify the

presence of transition layer when the maximum value of ' $\mu$ ' is positive below the main inversion and the ratio of the maximum value of ' $\mu$ ' and its average below the main inversion is greater than 1.3 (Yin & Albrecht, 2000). Note that ' $\theta$ ' is the potential temperature, 'r' is the mixing ratio, and 'P' is the atmospheric pressure.



Figure S3: Time-height cross-section with 1 min temporal resolution of Mean Doppler Velocity for (a) CAPRICORN and (b) control simulation. Data is analyzed for the entire case study period (26<sup>th</sup> of March 2016 at 00:00:00 UTC to 28<sup>th</sup> of March 2016 at 00:00:00 UTC).



Figure S4: Along the ship track, all the continuous reflectivity streaks which are passing through the reflectivity bins enclosed by the white rectangles in (b),(d),(f),(h) are plotted with distinct coloured lines for (a),(e) CAPRICORN and (c),(g) control simulation. The number of streaks passing through each reflectivity-height bin is normalized with the total number of streaks passing through the white box (given in percentage - that shows how the streaks are distributed across the various bins) for (b),(f) CAPRICORN and (d),(h) 1M.90ND, with the total number of data for each height bin is shown on right. The reflectivity inside a certain height bin abruptly changes when the data across the reflectivity bins in that height bin exceeds 100%. Data is analyzed for the entire case study period ( $26^{\text{th}}$  of March 2016 at 00:00:00 UTC to  $28^{\text{th}}$  of March 2016 at 00:00:00 UTC).



Figure S5: The two-day track (black) from CAPRICORN is offset  $(0.2^{\circ}E, 0.2^{\circ}S; 0.2^{\circ}W, 0.2^{\circ}N)$  for each track) to 10 different locations (green) for quasi-ensemble analysis.

![](_page_35_Figure_4.jpeg)

Figure S6: Normalized contoured frequency by altitude diagram with 1-min resolution for the quasi-ensemble control simulation.

![](_page_36_Figure_0.jpeg)

Figure S7: The spread of accumulated precipitation data for CAPRICORN, control simulation with data averaged for 2 km radius (1M.90ND) along the ship track and point data along the ship track at 10 different locations. The data from the track with no offset corresponds to 0°\_Offset. The accumulated precipitation is analyzed in the tracks shifted to the south-east (0.2°\_Offset, 0.4°\_Offset, 0.6°\_Offset, 0.6°\_Offset, 0.8°\_Offset and 1.0°\_Offset) and the north-west (-0.2°\_Offset, -0.4°\_Offset, -0.6°\_Offset, -0.8°\_Offset and -1.0°\_Offset) directions. Data is analyzed for the entire case study period (26<sup>th</sup> of March 2016 at 00:00:00 UTC to 28<sup>th</sup> of March 2016 at 00:00:00 UTC).

![](_page_37_Figure_2.jpeg)

Figure S8: Time-height cross-section of simulated radar reflectivity with 1 min temporal resolution for (a) 1M.20ND, (b) 2M.P (c) 2M.HM and (d) 2M.HM.BR03. Case study period: 26<sup>th</sup> of March 2016 at 00:00:00 UTC to 28<sup>th</sup> of March 2016 at 00:00:00 UTC.

![](_page_38_Figure_1.jpeg)

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(a)

300

250

(°- *mg*) 150 100 (°- *mg*) 100

50

![](_page_38_Figure_2.jpeg)

Figure S9: Spatial and temporal mean response obtained for the domain and case period of simulation in (a) IWP (all solid hydrometeors), (b) GWP, (c) ice number concentration (all solid hydrometeors), and (d) graupel number concentration. Domain is clipped around the ship track (see section 2.3).

![](_page_39_Figure_1.jpeg)

Figure S10: Spatial and temporal mean of ice microphysical processes for the entire simulation period ( $26^{\text{th}}$  of March 2016 at 00:00:00 UTC to  $28^{\text{th}}$  of March 2016 at 00:00:00 UTC).

![](_page_40_Figure_1.jpeg)

Figure S11: Time-height cross-section of simulated cloud-precipitation phase with 1 min temporal resolution for (a) 1M.20ND, (b) 2M.P (c) 2M.HM and (d) 2M.HM.BR03. Case study period: 26<sup>th</sup> of March 2016 at 00:00:00 UTC to 28<sup>th</sup> of March 2016 at 00:00:00 UTC.

![](_page_41_Figure_1.jpeg)

Figure S12: Spatial and temporal mean of graupel microphysical processes rates (solid lines). Dashed lines correspond to mean cloud base height. Blue and red lines represents 1M.90ND and 2M.HM simulation respectively. Shading corresponds to 20 to 80 percentile of CBH. The hourly data is processed only on 27<sup>th</sup> of March 2016.

Hydrometeor	1M.20ND (dBZ)	1M.90ND (dBZ)	2M.P (dBZ)	2M.HM (dBZ)	2M.HM.BR03 (dBZ)
All (normalized)	3.37	4.01	2.19	2.28	2.13
Àll	3689	3884	2174	2008	2060
Cloud water	1604	1822	579	254	367
Cloud ice	0	0	0	1296	1230
Rain	743	31	1940	921	973
Snow	3	16	0	942	1109
Graupel	3478	3665	612	756	750
Hail	-	-	10	0	0
(b)					
Hydrometeor	1M.20ND (%)	1M.90ND (%)	2M.P (%)	2M.HM (%)	2M.HM.BR03 (%)
Cloud water	27.52	32.92	18.43	6.09	8.29
Cloud ice	0	0	0	31.09	27.77
Rain	12.74	0.56	61.76	22.09	21.96
Snow	0.05	0.29	0	22.59	25.03
Graupel	59.68	66.23	19.48	18.13	16.93
Hail	-	-	0.32	0	0
(c)					
Hydrometeor	1M.20ND	1M.90ND	2M.P	2M.HM	2M.HM.BR03
	(%)	(%)	(%)	(%)	(%)
All	-5.02	-	-44.03	-48.30	-46.96
Cloud water	-11.96	-	-68.22	-86.06	-79.86
Rain	2296.77	-	6158.06	2870.97	3038.71
Snow	-81.25	-	-100	5787.50	6831.25
Graupel	-5.10	-	-83.30	-79.37	-79.54

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(a)

Table S1: Simulated bridge reflectivity analysis for the CFAD structure (-25 to 0 dBZ; 1.6 to 2 km altitude). (a) Sum of the reflectivities, (b) Percentage contribution of reflectivity of each hydrometeor with respect to the sum of individual reflectivities in every experiment and (c) Change in percentage compared to the control simulation (1M.90ND).

Experiment	Median (mm)	$25^{\text{th}}$ percentile (mm)	$75^{\text{th}}$ percentile (mm)
CAPRICORN	1.39	0.24	2.12
$2 \mathrm{km}$	0.68	0.03	2.07
0 deg	0.59	0.01	2.06
0.2	0.26	0.04	0.89
0.4	0.95	0.25	1.11
0.6	0.82	0.07	2.35
0.8	3.81	1.28	5.66
1	4.10	1.50	5.50
-0.2	0.98	0.05	1.28
-0.4	1.54	0.06	1.72
-0.6	2.41	0.15	4.50
-0.8	0.76	0.29	1.44
-1	0.14	0.08	1.53

Table S2: The median, 25<sup>th</sup> percentile and 75<sup>th</sup> percentile of accumulated precipitation for CAPRICORN in the first row and the control simulation in all other rows. A mean value of precipitation within a 2 km radius is calculated in 1M.90ND for each coordinate along the ship track (Experiment '2km'). The point-wise precipitation data are retrieved for all other tracks (Experiment '0deg' to '-1'), with the number reflecting the degree of offset and the south-east offset being regarded a positive direction and the north-west offset being considered a negative direction.

Hydrometeor	Below_freezing_line		Above_freezing_line	
	min	max	min	max
All	-40	20	-40	0.2
Cloud water	-40	-6.6	-40	-6
Ice	-	-	-40	-25.4
Rain	-40	20	-40	-1.6
Snow	-	-	-40	-13.7
Graupel	-40	4	-40	3.8

Table S3: The reflectivity range (dBZ) for each hydrometeors for control simulation. The row 'All' represents when all the hydrometeors are active in reflectivity calculation. The tentative freezing line has been set at 1.2 km.

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