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# Dynamical conditions of ice supersaturation and ice nucleation in convective systems: A comparative analysis between in situ aircraft observations and WRF simulations

John D'Alessandro San Jose State University

Minghui Diao San Jose State University, minghui.diao@sjsu.edu

Chenglai Wu University of Wyoming

Xiaohong Liu University of Wyoming

Ming Chen

See next page for additional authors

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#### Authors

John D'Alessandro, Minghui Diao, Chenglai Wu, Xiaohong Liu, Ming Chen, Hugh Morrison, Trude Eidhammer, Jorgen Jensen, Aaron Bansemer, Mark Zondlo, and Joshua DiGangi

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- 1 Dynamical conditions of ice supersaturation and ice nucleation in convective systems: a 2 comparative analysis between in-situ aircraft observations and WRF simulations
- 3 John J. D'Alessandro<sup>1</sup>, Minghui Diao<sup>\*1</sup>, Chenglai Wu<sup>2,3</sup>, Xiaohong Liu<sup>2</sup>, Ming Chen<sup>4</sup>, Hugh
- 4 Morrison<sup>4</sup>, Trude Eidhammer<sup>5</sup>, Jorgen B. Jensen<sup>6</sup>, Aaron Bansemer<sup>4</sup>, Mark A. Zondlo<sup>7</sup>, Josh P.
- 5 DiGangi<sup>8</sup>
- 6 <sup>1</sup>Department of Meteorology and Climate Science, San Jose State University, San Jose, CA,
- 7 USA, 95192-0104
- <sup>2</sup>Department of Atmospheric Science, University of Wyoming, Laramie, WY, USA, 82071.
- 9 <sup>3</sup>International Center for Climate and Environment Sciences, Institute of Atmospheric Physics,
- 10 Chinese Academy of Sciences, Beijing, China, 1000294
- <sup>4</sup>Mesoscale & Microscale Meteorology Division, National Center for Atmospheric Research,
- 12 Boulder, CO, USA, 80301
- <sup>5</sup>Research Applications Laboratory, National Center for Atmospheric Research, Boulder, CO,
   USA, 80301
- <sup>6</sup>Research Aviation Facility, National Center for Atmospheric Research, Broomfield, CO, USA,
  80021
- <sup>17</sup> <sup>7</sup>Department of Civil and Environmental Engineering, Princeton University, Princeton, NJ, USA,
- 18 08544
- <sup>8</sup>Chemistry and Dynamics Branch, NASA Langley Research Center, Hampton, VA, USA, 23666
- 20 \*Corresponding author:
- 21 Minghui Diao, Assistant Professor
- 22 Department of Meteorology and Climate Science, San Jose State University
- 23 One Washington Square, San Jose, CA 95192-0104
- 24 Minghui.diao@sjsu.edu; Phone: 609-933-6665

#### 25 Key points:

- 26 Ice supersaturation (ISS) occurrence frequencies in simulations show greater dependence on
- 27 vertical velocity than observations
- 28 Cooper parameterization of ice crystal formation suppresses ISS magnitude and frequency
- 29 Model-observation comparison results show improvements by limiting ice nucleation at lower
- 30 ISS

#### 31 Abstract

Occurrence frequency and dynamical conditions of ice supersaturation (ISS, where relative humidity with respect to ice (RHi) > 100%) are examined in the upper troposphere around convective activity. Comparisons are conducted between in-situ airborne observations and the Weather Research and Forecasting model simulations using four double-moment microphysical schemes at temperatures  $\leq -40^{\circ}$ C.

All four schemes capture both clear-sky and in-cloud ISS conditions. However, the clear-sky 37 (in-cloud) ISS conditions are completely (significantly) limited to the RHi thresholds of the 38 Cooper parameterization. In all of the simulations, ISS occurrence frequencies are higher by ~3– 39 4 orders of magnitude at higher updraft speeds (>  $1 \text{ m s}^{-1}$ ) than those at the lower updraft speeds 40 when ice water content (IWC) > 0.01 g m<sup>-3</sup>, while observations show smaller differences up to 41  $\sim$ 1–2 orders of magnitude. The simulated ISS also occurs less frequently at weaker updrafts and 42 downdrafts than observed. These results indicate that the simulations have a greater dependence 43 on stronger updrafts to maintain/generate ISS at higher IWC. At lower IWC ( $\leq 0.01$  g m<sup>-3</sup>), 44 45 simulations unexpectedly show lower ISS frequencies at stronger updrafts. Overall, the Thompson aerosol-aware scheme has the closest magnitudes and frequencies of ISS > 20% to the 46 47 observations, and the modified Morrison has the closest correlations between ISS frequencies and vertical velocity at higher IWC and number density. The Cooper parameterization often 48 49 generates excessive ice crystals and therefore suppresses the frequency and magnitude of ISS, indicating that it should be initiated at higher ISS (e.g.,  $\geq 25\%$ ). 50

#### 51 **1. Introduction**

52 Cirrus clouds cover approximately 30% of Earth at any given time [*Wylie and Menzel*, 1999], 53 and the global coverage of cirrus clouds plays a critical role in the global radiative budget [*Liou*, 54 1986; *Chen et al.*, 2000]. The microphysical properties of cirrus clouds play a critical role in 55 their radiative properties. These properties consist of ice particle mass, number concentration, 56 size distributions, as well as particle shape and surface roughness. An important factor that 57 directly affects the initiation of ice crystal formation as well as the microphysical properties is 58 the distribution of relative humidity with respect to ice (RHi). 59 Ice supersaturation (ISS) occurs when the ambient vapor pressure exceeds the saturation vapor pressure with respect to ice (i.e., ISS = RHi - 100%). The formation of ice clouds requires 60 the ambient conditions to be supersaturated with respect to ice. Unlike warm clouds, which are 61 composed entirely of liquid and develop when a fractional amount of supersaturation with 62 respect to water exists, ice cloud formation will not necessarily take place given the precondition 63 of ISS [e.g., Heymsfield et al., 1998; Gierens et al., 1999; Spichtinger et al., 2003; Peter et al., 64 2006; Krämer et al., 2009; Diao et al., 2014]. A critical relative humidity is often established to 65 predict the onset of homogeneous nucleation, based on the water activity of the solution [Koop et 66 al., 2000]. Concerning heterogeneous nucleation, ice nuclei (IN) can effectively nucleate ice 67 particles depending on temperature, RHi, and the physical and chemical properties of the IN 68 [Heymsfield and Miloshevich, 1995; Pruppacher and Klett, 1996; DeMott et al., 2011]. The 69 magnitudes of the ambient RHi can also impact size and number concentrations of ice particles 70 formed via both homogeneous and heterogeneous nucleation. 71

72 Anvil cirrus clouds are generally composed entirely of ice and are associated with upperlevel outflow during episodes of convective activity. Three factors are often involved in the 73 74 processes affecting the microphysical properties of anvil cirrus: RHi, the occurrence of preexisting ice particles, and vertical velocity [Heymsfield et al., 2005]. Vertical velocity is 75 76 important to consider due to rising (sinking) air associated with temperature decrease (increase) as a consequence of adiabatic expansion (compression). Therefore, an examination of vertical 77 velocity is necessary to correctly characterize temperature fluctuations and cooling/heating rates. 78 A notable positive relationship between updraft speeds and RHi has been reported for some time 79 80 [Heymsfield, 1977]. Previous studies using composite observations at various vertical levels have suggested temperature to be the most important factor in initiating ISS in the upper troposphere, 81 whereas fluctuations of water vapor are of secondary importance [Kärcher and Haag, 2004]. 82 More recently, analyses utilizing in-situ flight observations showed that by further restricting the 83 analysis to quasi-isobaric levels, water vapor spatial heterogeneities are the dominant factor that 84 determines the locations and magnitudes of ISS rather than temperature spatial heterogeneities 85 [*Diao et al.*, 2014]. 86

Recently, a study utilizing a box model analyzed the time evolution of ice microphysical
properties in relation to various constant background vertical velocities [*Krämer et al.*, 2016].

The study found that modifying the vertical velocities from  $0-3 \text{ m s}^{-1}$  can significantly impact 89 the evolution of RHi, ice water content (IWC), the effective radius (r<sub>e</sub>), and number 90 91 concentration (Nc) of ice particles, with the resulting IWC, re, and Nc varying by several orders of magnitude. Other studies have also investigated the competition between various ice 92 93 nucleation and freezing modes, and their impacts on properties such RHi, IWC and Nc [e.g., Gierens, 2003; Eidhammer et al., 2009; Barahona and Nenes, 2009]. Gierens [2003] used a box 94 95 model and showed that whether heterogeneous or homogeneous freezing dominates is determined by temperature, updraft speed, ambient pressure, and ISS. The author noted that 96 vertical velocity could differentiate whether heterogeneous or homogeneous nucleation would 97 occur, with stronger updrafts (on the order of 0.1 m s<sup>-1</sup> for pristine conditions to 1 m s<sup>-1</sup> for 98 polluted conditions) generally associated with homogeneous nucleation. The significance of 99 vertical velocity as a diagnostic parameter for ice microphysical properties, however, is still 100 uncertain. Muhlbauer et al. [2014] analyzed in-situ observations of ice microphysical properties 101 of cirrus clouds formed by various synoptic conditions and found that the probability density 102 functions (PDFs) of vertical velocity perturbations were similar amongst cirrus associated with 103 strong convection (anvil cirrus), frontal lifting around midlatitude cyclones, and upper-level 104 ridges, while particle size distributions were found to have distinct differences associated with 105 106 these mesoscale or synoptic conditions. Because of this, they concluded that vertical velocity is a poor predictive parameter for ice cloud microphysical properties. 107

108 The purpose of this study is to evaluate the frequency and magnitude of the simulated ISS in the upper troposphere in the Weather Research and Forecasting (WRF) model and compare 109 110 results with in-situ observations. Previously, Diao et al. [2015] examined in-situ airborne observations of RHi in the upper troposphere/lower stratosphere over North America and found 111 the average occurrence frequencies of ISS to be  $\sim 1.5-2$  times greater on the anticyclonic side of 112 the polar jet stream compared with the cyclonic side. This study aims to similarly examine the 113 occurrence and magnitude of RHi in convective regions. Additionally, the sensitivity of ISS to 114 local cooling rates driven by adiabatic expansion is examined by directly relating ISS to vertical 115 velocity within convective cirrus, anvil cirrus, and surrounding convective systems. Examination 116 of the RHi – vertical velocity relationship at larger spatial scales is certainly warranted; however, 117 the purpose of this study is to examine this relationship at the microscale by comparing in-situ 118 observations and WRF simulations. We will mainly compare the correlations among ISS, 119

vertical velocity, and ice microphysical properties (i.e., IWC and Nc). Sensitivity tests to address whether the compared correlations represent general physical processes or show a strong dependence on spatial/temporal sampling are also discussed. Overall, our comparison results help to evaluate the general performance of various microphysics schemes in the WRF model.

#### 124 **2. Data and methodology**

#### 125 2.1 In-situ measurements

In-situ measurements were taken by the National Science Foundation (NSF)/National Center for Atmospheric Research (NCAR) Gulfstream-V (GV) research aircraft during the NSF Deep Convective Clouds and Chemistry (DC3) campaign. The DC3 campaign took place during May 18 – June 30 2012 at the following locations: northeastern Colorado, northern Alabama, west Texas, and central Oklahoma. The campaign's objective was to target areas of convective outflow in midlatitude regions, with a major focus on observing NO<sub>x</sub> production by lightning (Barth et al. [2015] provides a detailed description of the DC3 campaign).

A total of 22 flights were performed by the GV aircraft, each with one-second merged data 133 134 (~250 m horizontal scale for 1 Hz data) from a suite of instrumentation. Water vapor measurements were taken from the 25 Hz, open-path Vertical Cavity Surface Emitting Laser 135 136 (VCSEL) hygrometer. Water vapor measurements are averaged to 1 Hz for consistency with other measurements. The accuracy and precision of water vapor measurements are ~6% and  $\leq$ 137 1%, respectively. Ice water content (IWC) is derived from the Fast Two-Dimensional Optical 138 Array cloud probe (Fast-2DC), which uses high-speed electronics and a 64-element 25 µm-139 resolution diode array in order to shadow particles at the sampling speeds of the GV. To reduce 140 uncertainties, only the particles that shadow a minimum of three or more diodes (having a 141 diameter of 62.5 µm or more) are included in the dataset. The effects of shattered ice particles on 142 the exterior arms or inlet shields of cloud probes are potentially important when analyzing 143 144 airborne ice particle measurements [e.g., Jensen et al., 2009]. The Fast-2DC is equipped with anti-shattering tips to minimize these effects. However, there is no perfect solution to completely 145 eliminate shattering, as previously reported [Korolev et al., 2013]. This study focuses on IWC 146 when evaluating ice particle measurements, which should result in lower uncertainties from ice 147 particle shattering than number concentrations. The IWC is derived from diameter and number 148

concentration measured by Fast-2DC using equations from Brown and Francis [1995]. 149 Temperature measurements were taken by a Rosemount temperature probe with the accuracy and 150 151 precision of ~±0.3 K and ~0.01 K, respectively. Vertical velocity measurements were derived from a suite of instrumentation, including the Radome Gust Wind Package, pitot tubes, 152 temperature probe, inertial reference unit, and the differential Global Positioning System, which 153 has a precision of ~0.012 m s<sup>-1</sup> and accuracy of ~0.15 – 0.3 m s<sup>-1</sup>. According to an in-flight 154 intercomparison conducted by the NCAR Research Aviation Facility between the GV vertical 155 velocity measurements and the NCAR Laser Air Motion Sensor (LAMS) instrument, very good 156 agreement is shown between them. RHi is derived from water vapor mixing ratio, pressure, and 157 temperature following the calculations in Murphy and Koop [2005]. When combining the 158 159 uncertainties in water vapor and temperature measurements, the uncertainty of RHi for the sampling range of 233.15 K to 207 K is ~6.9%–7.4%. 160

#### 161 2.2 WRF simulations

The Advanced Research WRF model simulations (version 3.7) were run with four 162 microphysics schemes, Morrison et al. [2009], a modified Morrison, Thompson et al. [2008], and 163 Thompson and Eidhammer [2014] (hereafter referred to as Morrison, Morrison-125%, 164 Thompson, and Thompson-aerosol, respectively) using the Global Forecast System (GFS) 6-165 hourly 0.5°×0.5° initialization data. Each simulation has a parent domain (12 km horizontal grid 166 spacing) and a nested domain (2.4 km horizontal grid spacing) with 40 vertical levels and a 167 pressure top of 30 hPa (except for 70 hPa in Thompson-aerosol). Simulations were run starting 168 on 19 May 2012 at UTC 0000 for 30 hours. We also conducted 800 m horizontal grid spacing 169 nested domain simulations for all microphysics schemes and the sensitivity tests show no 170 significant impacts on our conclusions. The timesteps for the parent and two nested domains are 171 172 60, 12 and 4 seconds, respectively (except for Thompson-aerosol with 30, 6 and 2 seconds, respectively). Figure 1 A shows the parent and nested domains, as well as the DC3 flight paths. 173 The Kain-Fritsch convective scheme [Kain, 2004] was only used in the parent domain. 174 Additionally, the physics options used in both the parent and nested domains of the four 175 simulations were the Dudhia shortwave radiation [Dudhia, 1989], the Rapid Radiative Transfer 176 Model (RRTM) longwave radiation [Mlawer et al., 1997], the Noah land surface model [Chen 177

*and Dudhia*, 2001], and the Mellor-Yamada-Janjic planetary boundary layer scheme [*Janjić*,
179 1994].

Both Morrison and Thompson include number concentrations of newly formed ice crystals 180 predicted by the Cooper [1986] parameterization, which is solely a prognostic function of 181 temperature,  $Nc_i = 0.005 \exp[0.304 * (T_0 - T)]$ , where  $Nc_i$  is the number of ice crystals 182 initiated (L<sup>-1</sup>), T<sub>0</sub> is 273.15 K, and T is the ambient temperature in Kelvin. Morrison and 183 Thompson initiate the Cooper parameterization when RHi exceeds 108% and 125% (or when 184 185 liquid saturation is reached below 265.15 K and 261.15 K), respectively, while Thompsonaerosol does not include the Cooper parameterization. The only modification in Morrison-125% 186 187 is to increase the RHi threshold for initiating the Cooper parameterization from the default value (RHi of 108%) to RHi of 125%. Additional restrictions on the Cooper parameterization are 188 applied, for example, Morrison and Thompson restrict the number concentration of ice particles 189 formed via the Cooper parameterization to 500 L<sup>-1</sup> and 250 L<sup>-1</sup>, respectively, and the mass-190 weighted mean size of cloud ice may not exceed 300 µm in Thompson. Both Morrison and 191 Thompson also allow for homogeneous and heterogeneous freezing of cloud droplets and rain, 192 where heterogeneous freezing is parameterized following Bigg [1953] (for both schemes) and 193 homogeneous freezing occurs instantaneously at -40°C and -38°C, respectively. Frozen cloud 194 droplets and rain can potentially account for a significant portion of the total Nc of frozen 195 hydrometeors in and around convection systems, where liquid droplets can be lofted to the 196 homogeneous freezing level. The treatment of deposition/sublimation rates for ice and snow in 197 Morrison is similar to Harrington et al. [1995], Ferrier [1994] and Reisner et al. [1998], whereas 198 the calculations in Thompson are based on Srivastava and Coen [1992]. 199

200 Thompson-aerosol is similar to Thompson, but explicitly treats aerosols categorized as either "water friendly" (hygroscopic) or "ice friendly" (non-hygroscopic), allowing for the activation of 201 202 aerosols as both IN and cloud condensation nuclei, initialized with the climatological aerosol 203 dataset. As described in Thompson and Eidhammer [2014], deposition freezing (below water 204 saturation) is parameterized with Phillips et al. [2008], while immersion freezing (at or above water saturation) is now parameterized with DeMott et al. [2011]. Homogeneous nucleation of 205 206 the "water friendly" aerosols is parameterized with Koop et al. [2000]. At the temperatures considered in this study ( $\leq$  -40°C), the DeMott parameterization will not activate since 207

homogeneous nucleation initiates at lower RHi compared with the DeMott parameterization.
Thus, while the Cooper parameterization in the other three microphysics schemes implicitly
includes heterogeneous and homogeneous nucleation, Thompson-aerosol allows for explicit
simulations of the competition between heterogeneous and homogenous nucleation.

212 All four microphysics schemes allow for supersaturation with respect to ice, without applying the saturation adjustment to the ice hydrometeors. In addition, all microphysics 213 schemes calculate the saturation vapor pressure with respect to ice following Flatau et al. [1992]. 214 Differences in the calculated RHi between Murphy and Koop [2005] and Flatau et al. [1992] are 215 minimal, ranging from ~0% to 0.34% at the combined water vapor and temperature ranges 216 sampled by the DC3 observations at -40°C and -65.8°C. However, there are somewhat larger 217 differences in liquid saturation between Flatau et al. [1992] and Murphy and Koop [2005], so 218 that slightly higher RHi values of 1.17% - 15.75% and 1.14% - 6.42% occur at liquid saturation 219 in both the Thompson and Morrison simulations based on Flatau et al. [1992] compared to 220 221 Murphy and Koop [2005]. This explains the occurrence of a small number of points in the simulations with RHi exceeding the liquid saturation line calculated by Murphy and Koop 222 223 [2005].

Our main analyses are based on simulations over the Great Plains region on 19 May 2012, 224 during a convective episode throughout the area. The event was marked by several high wind (> 225 33 m s<sup>-1</sup>) and hail (diameter > 5 centimeters) reports stretching from Southern OK up to Western 226 IA. The GV took observations on this day over Oklahoma, where a squall line associated with 227 the high winds and large hail occurred. The event was marked by elevated instability and 228 widespread values of CAPE above 1000 J kg<sup>-1</sup> throughout most of the region. A composite 229 dataset for each simulation is obtained by combining outputs at four times, UTC 1800, 2100, 230 0000, and 0300 from 19-20 May 2012 (i.e., 1-10 pm local time on 19 May 2012). These outputs 231 are chosen from the simulations to obtain data sampled over nine hours of a convective episode, 232 which included multiple clusters of thunderstorms and a well-developed squall line in the 233 southern domain (see Figure 1 B). High water vapor concentrations from the WRF simulations 234 were found to have similar spatial distributions to those seen in the GOES-13 satellite imagery. 235 236 Sensitivity tests of another set of realistic case simulations (11–12 June 2012) are also examined,

which show consistent conclusions for the statistical distributions of ISS and its correlation withvertical velocity.

To visualize the RHi and vertical velocity (w) fields from the simulations, Figure 1 B-D 239 shows RHi and w spatial distributions for the entire nested domain using Thompson. At 300 hPa, 240 241 gravity waves are seen surrounding the strongest updrafts and downdrafts, and ISS is often collocated with relatively high fluctuations in w (e.g., between 100°W–95°W) (Figure 1 B). The 242 vertical cross-section view at 40°N (Figure 1 C and D) reveals a deep convective structure with 243 w of  $\pm 5$  m s<sup>-1</sup> extending from 875 hPa to 250 hPa. The higher RHi (e.g., > 140%) appears to 244 occur almost exclusively at the upper tropospheric levels within regions of strong updrafts, while 245 weaker updrafts (e.g.,  $w > 0.5 \text{ m s}^{-1}$  at 97°W near 300 hPa) also collocate with RHi > 130%. 246

#### 247 2.3 Composite datasets for the comparisons between observations and simulations

248 To conduct the comparison, similar restrictions are imposed on the composite datasets for insitu observations (1 Hz data from 22 flights) and WRF simulations (all grid points in the nested 249 domain for four time outputs). Data analyses are restricted to regions where the temperature is 250 less than or equal to -40°C to prevent the sampling of mixed-phase clouds for the purposes of 251 solely analyzing the distributions of RHi and microphysical properties of ice particles. The 252 minimum IWC reported for one particle per 1 Hz measurements from the Fast-2DC probe in the 253 DC3 campaign is used to define in-cloud conditions in both observations and simulations (i.e., 254 IWC  $\ge 3.82 \times 10^{-5}$  g m<sup>-3</sup>), whereas clear-sky conditions are defined when IWC is less than this 255 threshold. The four microphysics schemes considered in this study predict mass mixing ratios for 256 three types of frozen hydrometeors: ice, snow, and graupel. For the simulations, IWC is treated 257 258 as the sum of these quantities. Similarly, Nc is treated as the total number of the frozen hydrometeors. Morrison and Morrison-125% predict Nc for ice, snow, and graupel, whereas 259 Thompson and Thompson-aerosol only predict Nc for ice. The observational data are restricted 260 to below the tropopause, where the tropopause height is based on the National Centers for 261 Environmental Prediction (NCEP) GFS-FNL (final) dataset interpolated onto the GV aircraft 262 position and time. Simulation datasets are restricted to regions where ambient pressure  $\geq 148$ 263 hPa (i.e., the lowest pressure sampled by GV in DC3). With these restrictions imposed, the total 264 number of 1 Hz observations in 22 flights amounts to  $\sim 67$  hr, compared with  $\sim 10^6$  of grid points 265 266 in the 2.4 km nested domain for four time outputs. We also examined the correlations between

ISS probabilities and w by using the in-situ observations onboard the NASA DC8 research aircraft during the DC3 campaign, and found consistent correlations between ISS frequencies and w as those shown in the composite dataset from the GV aircraft.

270 **3. Results** 

271 3.1 RHi distributions at various temperatures for clear-sky and in-cloud conditions

272 Occurrences of RHi are shown for both in-cloud and clear-sky conditions (Figure 2 left two columns). Throughout the entire temperature distribution shown for the observations, RHi ranges 273 274 from ~10% to as high as 160% and 150% for in-cloud and clear-sky conditions, respectively. The few occurrences of RHi above the liquid saturation line are within the range of measurement 275 276 uncertainties. Similar to the observations, the simulated in-cloud RHi most frequently occur within  $\pm 5\%$  to  $\pm 15\%$  of ice saturation, yet they all extend to higher values (RHi around 180%) 277 278 compared with the observations. Additionally, all of the simulations show a slight increase in 279 RHi occurrences around the liquid saturation line, which may be attributed to regions near and within the convective core of deep convective systems (as illustrated in Figure 1 B–D), where 280 aircraft would avoid sampling due to strong turbulence. Previously, simulations of an idealized 281 squall line scenario without synoptic scale dynamic forcings and radiative forcings did not 282 capture ISS at clear-sky conditions [Diao et al., submitted]. Thus, the capability of capturing ISS 283 at both clear-sky and in-cloud conditions in the WRF simulations suggests that larger-scale 284 dynamical forcings and/or radiative forcings play an important role in ISS formation. 285

The unrealistic limits of the clear-sky RHi magnitudes in Morrison, Morrison-125% and 286 287 Thompson are also the respective RHi thresholds for initiating the Cooper parameterization (i.e., RHi of 108%, 125%, and 125%, respectively). Similarly, sharp gradients are seen for in-cloud 288 289 RHi distributions. In comparison, Thompson-aerosol without the Cooper parameterization shows clear-sky ISS extending to the liquid saturation line, with ISS as high as ~60% occurring at 290 291 colder temperatures. By increasing the default threshold of initiating the Cooper parameterization, Morrison-125% produces more comparable results to the observations than the 292 293 default Morrison in terms of the magnitude and frequency of ISS allowed at the relatively higher 294 RHi (> 108%).

295 The PDFs of RHi are compared among observations and four individual WRF time outputs (Figure 2 right two columns). For in-cloud conditions, the PDF of RHi for DC3 dataset centers at 296 297 ~100%, which is consistent with previous in-situ observations of in-cloud RHi distributions [Ovarlez et al., 2002; Krämer et al., 2009; Diao et al., 2014]. Morrison, Thompson and 298 Thompson-aerosol all have much higher in-cloud RHi probabilities ( $\sim 0.16 - 0.18$ ) centered at ice 299 saturation compared with that of observations ( $\sim 0.09$ ), while Morrison-125% has the most 300 comparable RHi frequency (~0.1) at ice saturation. The variations in RHi distributions with 301 respect to different time outputs appear minimal for the simulations, where the most notable 302 change are the narrower peaks of PDF centered at RHi = 100% along the time evolution. 303 Thompson-aerosol is the only scheme that allows for noticeable RHi probabilities at RHi > 304 125% as seen in the observations, especially for the earlier time outputs, even though this 305 scheme shows slightly higher probabilities (e.g.,  $\sim 0.01-0.02$  at RHi = 130%) at this RHi range 306 than those in the observations ( $\sim 0.01$  at RHi = 130%). 307

308 For clear-sky conditions, PDFs of RHi for the simulations and observations both peak around 10%. However, the decay of RHi frequency from RHi of 20% to 80% is much sharper in all the 309 simulations, while the RHi frequency appears almost constant from 40%-80% in the 310 observations. In addition, observations show higher probabilities of clear-sky ISS than 311 312 simulations, with Thompson-aerosol having the highest clear-sky ISS frequency amongst the simulations. These discrepancies between observations and simulations may be subject to 313 sampling differences between DC3 and WRF, since the GV aircraft often sampled regions within 314 24 hours of convective activity, whereas the entire nested domain of WRF simulations is 315 included in the datasets (as shown in Figure 1). However, we note that the lack of clear-sky ISS 316 occurrence frequencies in the simulations is not necessarily due to a lack of clear-sky sampling. 317 In fact, the total number of samples (i.e. 1 Hz data and grid points) for in-cloud and clear-sky 318 conditions are proportionally about 1:2 in DC3 and about 1:7 in the WRF simulations. 319

320 3.2 Temperature, vertical velocity, IWC, and Nc distributions inside ISS conditions

The normalized frequency distributions of temperature, w, IWC and Nc are shown for various ranges of ISS (Figure 3 A–D and E–H). Temperature distributions of the four simulations are similarly well dispersed, whereas observations sampled more frequently at  $-50^{\circ}$ C to  $-46^{\circ}$ C than at  $-46^{\circ}$ C to  $-40^{\circ}$ C. 325 The PDFs of w for in-cloud (clear-sky) ISS conditions (Figure 3 C and D) are centered at 0.34 m s<sup>-1</sup> (-0.02 m s<sup>-1</sup>) and ~0.14 m s<sup>-1</sup> (~0.01 m s<sup>-1</sup>) for observations and simulations, 326 327 respectively, showing a slightly higher average w for in-cloud ISS in the observations. The cumulative frequency distributions (CFDs) of w for in-cloud ISS (Figure 3 E) show strong 328 329 sensitivities to ISS magnitudes in Morrison and Morrison-125%, with their 90th percentile of w increases from 0.25 m s<sup>-1</sup> to 1–2 m s<sup>-1</sup> when ISS increases from below to above 20% (Figure 3 330 E). For clear-sky conditions, the CFDs of w are similar between the observations and simulations 331 for different ISS ranges (> 20% and < 20%) (Figure 3 F). This suggests that vertical velocity, as 332 a parameter, may be a poor predictor for the magnitude of clear-sky ISS. Standard deviations of 333 ~0.9 m s<sup>-1</sup> are seen for all the simulations compared to ~0.57 m s<sup>-1</sup> in the observations as a result 334 of the intense updrafts and downdrafts sampled in simulations (up to ~50 m s<sup>-1</sup> in Morrison and 335 Morrison-125%, ~40 m s<sup>-1</sup> in Thompson and Thompson-aerosol, and as low as ~ -17 m s<sup>-1</sup> in all 336 the simulations). 337

338 Large differences in IWC and Nc distributions exist among the observations and simulations for different ranges of ISS. In Morrison, the IWC distribution peaks at ~0.025 g m<sup>-3</sup> for ISS  $\leq$ 339 20%, and this peak shifts to a significantly larger value at ~2.5 g m<sup>-3</sup> for ISS > 20%, which is 340  $\sim$ 1.5 orders of magnitude greater than that in the observations (Figure 3 G). Thompson-aerosol 341 has the opposite trend compared with Morrison, as it shows a decreasing IWC trend with 342 increasing ISS magnitudes. In addition, the average Nc in Thompson-aerosol decreases by more 343 344 than a factor of 4 from ISS  $\leq 20\%$  to ISS > 20%. In fact, Thompson-aerosol is the only scheme that shows both decreasing IWC and Nc with increasing ISS, similar to the observations. 345

Consequences of the different IWC and Nc distributions among the various simulations can 346 be seen in the CFDs of w for in-cloud ISS conditions. When higher IWC and/or Nc exist, higher 347 348 w are often seen to be associated with in-cloud ISS conditions. For in-cloud ISS > 20%, Morrison and Thompson-aerosol have ~20% and 80% of w below 0.25 m s<sup>-1</sup>, respectively, likely 349 due to the higher IWC and Nc values in Morrison. These results are consistent with the previous 350 351 theoretical calculations, which showed that ice cloud properties can significantly impact the incloud ISS distributions due to the depositional growth of ice crystals [Kärcher 2012]. Thus, it is 352 crucial to account for in-cloud properties (e.g., IWC and Nc) when evaluating the impacts of 353 various magnitudes of vertical velocity on the characteristics of ISS. 354

#### 355 3.3 Average vertical velocities for in-cloud ISS conditions

Analysis of average w for in-cloud conditions associated with various magnitudes of ISS is 356 shown in Figure 4. The factors of IWC and Nc are separately accounted for (on the y-axis of 357 Figure 4) in order to appropriately evaluate the impacts of various magnitudes of w on ISS. The 358 359 average w is calculated within each bin of log-scale IWC (or Nc) for various ranges of ISS. To examine the potential effects of ice shattering artifacts in the observational dataset, additional 360 analysis excluding ice particles smaller than 100 µm is shown (Figure 4, panel A3), which is 361 consistent with the observations including particles  $\geq 62.5 \ \mu m$  (panel A2). We note that since 362 the simulations include all frozen hydrometeors extending to size of zero, the Nc in observations 363 would have a low bias due to the lack of small particles, while the IWC comparisons dominated 364 by larger particles would be less affected. 365

For observations, the average w increases with the increasing IWC and Nc when they exceed 366 0.001 g m<sup>-3</sup> and 1 L<sup>-1</sup>, respectively. Such increases in the average w with IWC or Nc become 367 even greater as the magnitudes of ISS increase. For simulations, at IWC > 0.01 g m<sup>-3</sup> or Nc > 368 100 L<sup>-1</sup>, the differences in the average w for the various magnitudes of ISS are much larger (i.e., 369 by  $\sim 1-15$  m s<sup>-1</sup>) than those in the observations (by  $\sim 0.2-1$  m s<sup>-1</sup>). Thus, both observations and 370 simulations show that on average the presence of higher updrafts are required to initiate/maintain 371 372 the higher magnitudes of in-cloud ISS when associated with relatively high IWC (or Nc), yet the average w in simulations is even higher at the same magnitudes of in-cloud ISS. Note that the 373 Morrison simulation does not have IWC <  $10^{-3}$  g m<sup>-3</sup> or Nc < 300 L<sup>-1</sup> at RHi  $\ge$  108%, due to the 374 initiation of ice crystal formation from the Cooper parameterization. In addition, as the only 375 scheme that does not include the Cooper parameterization, Thompson-aerosol is the only 376 simulation that captures the low values of IWC (i.e.,  $\sim 3 \times 10^{-5}$  g m<sup>-3</sup>) and Nc ( $\sim 0.01$  L<sup>-1</sup>) for each 377 interval of ISS shown. 378

379 3.4 Correlations between the probabilities of ISS and w for in-cloud conditions

To examine the physical processes controlling ISS formation in the WRF simulations, we compare the simulated correlations between ISS probabilities and w with those from observations for in-cloud conditions (Figures 5 and 6). The comparisons between observations and simulations in Figures 5 and 6 are restricted to the same ranges of w, which exclude the

extreme updrafts and downdrafts sampled in the simulations but not in the observations as 384 discussed prior (Figure 3). By restricting the analysis to the same ranges of w, we avoid sampling 385 biases in w for the comparisons. Probabilities of ISS are calculated for each given range of w, 386 that is, the number of occurrences of ISS (within a given 10% interval) are normalized by the 387 total number of occurrences at all RHi ranges for the given range of w. We also control the 388 factors of IWC and Nc because of their potential influences on ISS characteristics. That is, the 389 390 ISS probabilities are calculated for various scales of w within individual bins of IWC (Figure 5) and Nc (Figure 6). 391

For the correlations between ISS probabilities and w, observations show that the probabilities 392 of ISS < 10% are relatively similar for various ranges of w given the same ranges of IWC or Nc 393 (except for a few larger IWC and Nc values). In contrast, all the simulations show decreasing 394 probabilities of ISS < 10% correlated with increasing w. For the higher ISS  $\geq$  10%, 395 observations show higher ISS probabilities in the stronger updrafts than weaker updrafts or 396 downdrafts. The increases in ISS probabilities from weaker to stronger updrafts are even more 397 evident as IWC (or Nc) increases, indicating that stronger updrafts are generally required to 398 generate/maintain ISS when associated with higher IWC or Nc. 399

Compared with a consistent positive correlation between probabilities of ISS  $\ge 10\%$  and w 400 as shown in the observations, simulations show different correlations between IWC >  $0.01 \text{ g m}^{-3}$ 401 and IWC  $\leq 0.01$  g m<sup>-3</sup> (Figure 5). Note that Morrison does not have the lower IWC (< 0.01 g m<sup>-3</sup> 402 <sup>3</sup>) and lower Nc (< 300 L<sup>-1</sup>) at RHi > 108% due to the excess ice crystal formation from the 403 Cooper parameterization. At IWC > 0.01 g m<sup>-3</sup>, the main difference between the observations 404 and the other three simulations (Morrison-125%, Thompson, and Thompson-aerosol) is that the 405 simulations show much higher probabilities of ISS associated with relatively strong updrafts than 406 those with weak updrafts or downdrafts. In fact, the differences in the probabilities of ISS  $\geq$ 407 10% increase by 1-1.5 orders of magnitude from downdrafts and weaker updrafts to stronger 408 updrafts in the observations, while those in the simulations increase by 2–4 orders of magnitude. 409 Sensitivity tests on individual flights show consistent results where observations have smaller 410 411 differences in the probabilities of ISS between lower and higher w than the simulations.

412 Among the four simulations, Morrison-125% has minimal differences in ISS probabilities between higher and lower w below the RHi threshold of initiating the Cooper parameterization. 413 414 Such improvement in Morrison-125% cannot be accounted for by only adjusting the Nc upper limit in the scheme (the maximum-allowed concentration of ice). This is seen in Figure 5 row 3 415 with an additional simulation that changes this limit in the Morrison scheme (Nc  $< 500 \text{ L}^{-1}$ ) to 416 the value used in Thompson (Nc  $< 250 \text{ L}^{-1}$ ), while using the default RHi threshold of 108% 417 (named as Morrison-Nc250). At IWC  $\leq 0.01$  g m<sup>-3</sup>, simulations show that probabilities of ISS  $\geq$ 418 10% are surprisingly lower at relatively higher w (w > 0.5 m s<sup>-1</sup>) than those at the lower w, by 419  $\sim$ 0.5–1 orders of magnitude. These results indicate that compared with observations, simulations 420 421 have a greater dependence on stronger updrafts for generating and/or maintaining ISS  $\ge 10\%$  at the higher IWC values, while an opposite correlation between ISS probabilities and w are shown 422 in the simulations at the lower IWC values. A simulation with twice the number of vertical levels 423 424 (i.e., 80 levels) was conducted for the Thompson-aerosol scheme (named as Thom-aer-80lev), showing that the differences in the probabilities of ISS > 10% between lower and higher w are 425 still ~2-4 orders of magnitude. In addition, a slight increase in the probabilities of ISS in 426 downdrafts and weaker updrafts by ~0.5 order of magnitude is seen at relatively higher IWC and 427 428 Nc, suggesting that increasing the number of vertical levels allows for more ISS at lower w for in-cloud conditions. 429

Compared with the analysis controlling for IWC (Figure 5), the analysis controlling for Nc (Figure 6) shows smaller differences in ISS probabilities by 1–2 orders of magnitude between the higher and lower w in all of the simulations, which are comparable to the scales shown in the observations. Morrison-125% has increasing probabilities of ISS with increasing Nc for almost all ranges of w, while Thompson, Thompson-aerosol, and Thom-aer-80lev show decreasing ISS probabilities at higher Nc. Thom-aer-80lev has the most comparable results to the observed range of ISS probabilities among all of the simulations when controlling for Nc.

Higher resolution WRF simulations using the 800 m nested domain are further examined to evaluate the sensitivities of the simulated correlations between ISS probabilities and w to horizontal grid spacings (Figures 7 and 8). The overall correlations between ISS and w are consistent between the 2.4 km and 800 m horizontal grid spacing simulations, that is, the positive and negative correlations between ISS probabilities and w are consistently shown at IWC > 0.01 g m<sup>-3</sup> and IWC  $\leq 0.01$  g m<sup>-3</sup>, respectively. The differences between the two resolutions are mainly shown in the differences of ISS probabilities between higher and lower w. Compared with the 2.4 km simulations, the differences of the probabilities of ISS  $\geq 10\%$  in the 800 m simulations decrease (i.e., closer to observations) at higher IWC (> 0.01 g m<sup>-3</sup>) or Nc (> 10 L<sup>-1</sup>), but increase (i.e., more dissimilar to observations) at the lower IWC and Nc. These results suggest that increasing the model resolution does not necessarily produce more comparable results to the observations for all IWC and Nc ranges.

3.5 The normalized occurrence frequency of ISS at the full range of w in observations andsimulations

When comparing w at the same magnitudes sampled in observations and simulations in Figures 5–8, the full range of w sampled in WRF simulations is not shown. To provide a depiction of the full range of w for in-cloud conditions, the normalized occurrence frequencies of ISS are further analyzed in relation to all w values, with the factors of IWC and Nc controlled in Figures 9 and 10, respectively. The normalized ISS frequencies are calculated by normalizing the number of ISS data in each IWC–w bin (or Nc–w bin) with the total number of RHi data in that bin, and results are shown in four ranges of ISS from 0–10%, 10%–20%, 20%–30% to  $\geq$  30%.

In Figure 9, both observations and WRF simulations show increasing occurrence frequencies 458 of ISS at higher updraft speeds and larger IWC, and the higher ISS frequencies in stronger 459 460 updrafts are more prominent in the simulations than in the observations at IWC > 0.01 g m<sup>-3</sup>, which is consistent with the comparisons in Figures 5 and 7. At this IWC range, all the 461 simulations show larger increases in the frequencies of ISS  $\ge 20\%$  from near zero to ~0.3 as w 462 increases from 0 to 3 m s<sup>-1</sup>, while the observations show smaller increases in ISS frequencies 463 (from ~0.1 to ~0.2). In addition, when w is above 3 m s<sup>-1</sup>, all of the simulations show larger 464 frequencies of ISS  $\ge$  20% than those in the observations, while they also show lower ISS 465 frequencies in weaker updrafts and downdrafts (w < 0.5 m s<sup>-1</sup>). For weaker updrafts and 466 downdrafts, most of the simulated ISS is below 10% (Figure 9 first column), while only 467 Morrison and Morrison-125% allow ISS  $\ge 10\%$  in strong downdrafts (w < -2 m s<sup>-1</sup>). Thompson-468 aerosol is the only scheme that shows ISS frequencies greater than 0.1 at the lower IWC (< 0.01469

g m<sup>-3</sup>), since more ice crystals with higher IWC are likely generated due to the Cooper
parameterization in the other schemes.

Simulations also show stronger correlations between ISS and Nc than observations at Nc > 472 100 L<sup>-1</sup> (Figure 10), which is similar to those shown at IWC > 0.01 g m<sup>-3</sup>. In addition, a lack of 473 ISS occurrences at w < 0.5 m s<sup>-1</sup> is shown in all the simulations at ISS  $\ge$  10%, except for 474 Morrison-125%. One feature that is shown in Figure 10 but not in Figure 9 is that Thompson-475 aerosol has a peak ISS frequency at Nc around 0.1 L<sup>-1</sup>, likely due to the predicted heterogeneous 476 IN number concentration by the Phillips et al. [2008] parameterization. For the same purpose of 477 addressing the effects of potential ice particle shattering as discussed in Figure 4, results with 478 restricted Nc values (excluding ice particles smaller than 100 µm) are also provided. Similar 479 480 occurrence frequency distributions of ISS are shown in the observations with or without such restriction. 481

3.6 Examining the influences of different sampling methods, time outputs, and different casestudies

484 To examine the sensitivity of the relationship between ISS and w to the spatial/temporal sampling method, we analyze the normalized occurrence frequencies of ISS for the WRF gridded 485 data collocated with the observations during the May 19<sup>th</sup> flight (Figure 11 top three rows). WRF 486 gridded data were selected within certain spatial ranges of the in-situ observations in latitude and 487 longitude (i.e.,  $\pm 0.5^{\circ}$ ,  $\pm 1.5^{\circ}$ , and  $\pm 3.0^{\circ}$ ) and within a time window ( $\pm 30$  min). Six hourly outputs 488 were used for the collocated comparisons from May 19th, UTC 2100 to May 20th, UTC 0200. 489 The results are shown for the Thompson-aerosol aware simulation, while other microphysics 490 491 schemes show similar consistency when conducting the collocated comparisons. In addition, to examine whether the correlations between ISS and w vary with the time evolution of the 492 convective system as well as with different convective events, the normalized occurrence 493 frequencies of ISS are analyzed for three combined time outputs during a separate convective 494 episode on 11–12 June 2012 (Figure 11 bottom four rows). The domain of the 11–12 June 2012 495 simulations also coincided with flight observations during the DC3 campaign. This day was 496 marked by isolated thunderstorms over Missouri/Arkansas and a mesoscale convective system 497 over Alabama, both of which were sampled by the GV aircraft. 498

499 Overall, the two main differences between observations and simulations that are shown in the 19-20 May 2012 case (Figure 9) are also captured in these two sensitivity tests shown in Figure 500 501 11, that is, (1) a stronger gradient in ISS frequencies is shown in the simulations than observations at IWC > 0.01 g m<sup>-3</sup>, and (2) a lack of ISS occurrences at w < 0.5 m s<sup>-1</sup> is shown in 502 the simulations. In addition, Thompson-aerosol is still the only scheme that captures the ISS 503 frequencies > 0.1 associated with lower IWC values (< 0.01 g m<sup>-3</sup>) in the 11–12 June 2012 case, 504 even though it shows higher occurrence frequencies of ISS  $\ge 30\%$  at w > 1 m s<sup>-1</sup> than that in the 505 19-20 May 2012 case. These results indicate that the comparisons between observations and 506 simulations on the correlations between ISS occurrence frequencies and w do not vary 507 significantly by convective events arising from different synoptic/mesoscale forcings or by using 508 509 more restrictive sampling methods.

The normalized frequency distributions of ISS are further compared among different time 510 outputs of the same convective episode. Analyses on the four individual time outputs used in the 511 composite datasets of the 19-20 May 2012 case are shown for Morrison and Thompson (Figure 512 12). There is a noticeable evolution of the normalized frequencies of ISS from UTC 1800 to 513 UTC 0300, namely, the full range of w distributions increases from  $\pm 1 \text{ m s}^{-1}$  to greater than  $\pm 6$ 514 m s<sup>-1</sup> at ISS conditions. Nevertheless, the sharp gradient in ISS frequencies between stronger 515 updrafts ( $w > 0.5 \text{ m s}^{-1}$ ) and weaker updrafts are still visible amongst individual time steps. In 516 addition, the lack of ISS associated with  $w < 0.5 \text{ m s}^{-1}$  at high IWC values (> 0.01 g m<sup>-3</sup>) is also 517 consistently shown in these time outputs. These results indicate that even though the range of w 518 varies among different time outputs, the overall distributions of ISS frequencies, as well as their 519 correlations with w and IWC, are consistent regardless of the selection of time outputs for our 520 521 analysis.

#### 522 4. Discussions and conclusions

WRF simulations with the Morrison et al. [2009], modified Morrison, Thompson et al. [2008], and Thompson and Eidhammer [2014] microphysics schemes captured both in-cloud and clear-sky ISS. The Cooper parameterization for ice crystal formation is included in the first three schemes but not in Thompson-aerosol. Including or excluding the Cooper parameterization, as well as changing the RHi thresholds for initiating the Cooper parameterization, have large impacts on our analysis of RHi, IWC, and Nc. For RHi distributions at temperature  $\leq -40^{\circ}$  C 529 (Figure 2), Cooper parameterization restricts the frequency and magnitude of ISS in simulations compared with the observations, which is likely due to the high number concentrations of ice 530 particles being formed through this parameterization. By increasing the RHi threshold for the 531 Cooper parameterization from the default 108% to 125% in Morrison-125%, a significant 532 increase in the occurrences of RHi above 108% is shown. Additionally, the Cooper 533 parameterization restricts the simulations from having lower IWC or lower Nc values at larger 534 values of ISS. For example, Morrison does not have IWC < 0.01 g m<sup>-3</sup> or Nc < 100 L<sup>-1</sup> at ISS  $\geq$ 535 8%. Other microphysics schemes that predict ice nucleation as a function of temperature may 536 potentially yield similar discrepancies as produced via the Cooper parameterization. Thus, results 537 from this study suggest that the Cooper parametrization, if included, should be initiated at higher 538 RHi values (such as RHi  $\geq 125\%$ ) at temperatures  $\leq -40^{\circ}$ C. Given the simplicity of the Cooper 539 parameterization for more economical computations, adjusting the RHi threshold is found to be 540 most effective for improving the simulations of ISS and ice nucleation compared with modifying 541 other factors (e.g., Nc upper-limit, number of ice nuclei and vapor deposition rate) in both the 542 current study and another study [Diao et al., submitted]. Thus, the Cooper parameterization with 543 544 the adjustments recommended will still be valuable, and it does not involve the uncertainties of aerosol fields when using the Thompson-aerosol scheme. Based on these results, microphysics 545 schemes are recommended to consider limiting ice nucleation at lower ISS even at low 546 547 temperatures  $\leq$  -40°C. These results are consistent with the previous remote sensing studies focusing on warmer conditions (> -40°C) suggesting that ice nucleation is limited when RHi is 548 below water saturation [Ansmann et al., 2008; de Boer et al., 2011]. 549

Concerning correlations between ISS and w at various IWC (Nc) ranges, observations show a 550 consistent positive correlation between probabilities of ISS and w (Figures 5 and 6), suggesting 551 552 that higher w is generally required to generate and/or maintain the higher magnitudes of ISS. Such positive correlations between ISS probabilities and w are stronger when IWC or Nc 553 increases, or when ISS magnitudes increase. In contrast, two types of ISS - w correlations occur 554 in the simulations: a positive correlation at IWC > 0.01 g m<sup>-3</sup> (or Nc > 100 L<sup>-1</sup>) and a negative 555 correlation at lower IWC (or lower Nc). Although the simulations have a positive correlation 556 between ISS probabilities and w at higher values of IWC or Nc, such correlations are much 557 stronger in the simulations with differences in ISS probabilities up to 4 orders of magnitudes 558

between weak and strong updrafts (i.e.,  $0.1 - 4 \text{ m s}^{-1}$ ). In comparison, the differences in observations are only up to 2 orders of magnitude. The stronger dependence of ISS probabilities on w in the simulations for generating and/or maintaining ISS at IWC > 0.01 g m<sup>-3</sup> or Nc > 100 L<sup>-1</sup> is consistently shown in a series of analyses (Figures 5 – 8), and is also evident by the large increases of ISS frequencies from weaker to stronger updrafts in Figures 9 – 12. As a result of this strong dependence on w in the simulations, a lack of ISS is associated with weaker updrafts and downdrafts (w < 0.5 m s<sup>-1</sup>) at high IWC and Nc values in Figures 9 – 12.

The discrepancies in the correlations between ISS probabilities and w between the 566 567 observations and WRF simulations may be due to several factors. For in-cloud ISS, it is possible that the relaxation rate of ISS (i.e., the time for the existing ice to deplete the available water 568 vapor over ice saturation) may be excessive at higher IWC (or Nc), which would require stronger 569 updrafts to enhance the magnitudes of RHi as the excess water vapor is rapidly depleted at 570 relatively high IWC (or Nc). A series of previous studies have discussed the complex factors 571 572 influencing the vapor deposition rates, including studies on the spherical particles [Korolev and Mazin, 2003] and the non-spherical particles [Sheridan et al., 2009], as well as those on the 573 574 uncertainties with regard to the kinetically-limited growth [e.g., Harrington et al., 2009; Zhang and Harrington, 2015]. In addition, all the microphysics schemes in this study include 575 576 homogeneous (and heterogeneous) freezing of cloud droplets and rain, which can affect ice concentrations and ISS relaxation time below -40°C, especially in and near deep convection. 577 Thus, it is not just the representations of ice nucleation on aerosols (as opposed to activated 578 cloud droplets/rain) that can lead to differences between simulations and observations, although 579 580 large impacts are still seen in the ISS frequency and magnitude when modifying the Cooper parameterization threshold in Morrison-125%. 581

Another potential explanation for the different ISS – w correlations between the observations and simulations may be that the water vapor spatial heterogeneities on the cloud scale (~1 km) are not sufficiently resolved by the simulations. Water vapor spatial variabilities have been previously reported to be the dominant contributor to the variabilities of RHi for both clear-sky and in-cloud conditions compared with the spatial variabilities of temperature [*Diao et al.*, 2014]. One may argue that increasing the horizontal resolution of the WRF simulations would provide a better representation of the water vapor spatial heterogeneities. However, when reducing the horizontal grid spacing from 2.4 to 0.8 km, even though the ISS probabilities at various w ranges in all the simulations become closer to the observations at IWC > 0.01 g m<sup>-3</sup> (or Nc > 100 L<sup>-1</sup>), the simulations also show larger discrepancies compared with the observations for representing ISS probabilities at the lower ranges of IWC and Nc. More investigation, such as using a cloudresolving model [e.g., *Diao et al.*, submitted], is needed to examine if higher resolution simulations could help to produce more comparable results to the observations.

We caution that there are several caveats with the current analysis, mainly due to various 595 factors in addition to IWC and Nc that potentially influence ISS distributions, such as the 596 evolution of ISS and ice crystal regions [Diao et al., 2013]. The analysis of ISS, IWC, and Nc in 597 this study represents a composite dataset that sampled cirrus clouds at various evolution stages 598 (e.g., nucleation, growth, sedimentation). We examined the correlations between ISS frequencies 599 and w at various pressures and altitudes, and found that these two factors have smaller impacts 600 than those of IWC and Nc. Another potential impact on the formation of ISS is from the various 601 602 scales of dynamical processes, including smaller scale gravity waves and turbulence, and mesoscale to synoptic scale dynamical conditions, such as frontal uplifting, mesoscale gravity 603 604 waves, warm conveyor belts, and jet streams [Spichtinger et al., 2005a, 2005b; Muhlbauer et al., 2014; Diao et al., 2015]. Additional work is recommended to further distinguish how the 605 606 relationship between ISS and vertical velocity is represented by different cloud microphysics schemes in global climate models, where vertical velocity fluctuations associated with mesoscale 607 608 phenomenon are parameterized due to the sub-grid scale (< 100 km) nature of these fluctuations, as well as in smaller scale model simulations such as the WRF-Large Eddy Simulations. 609

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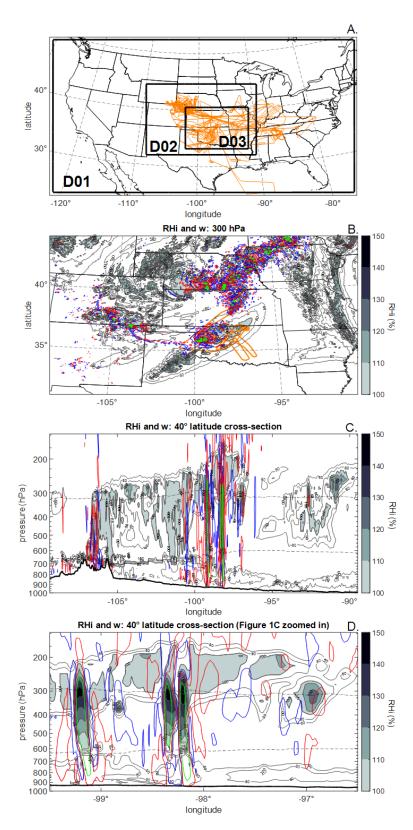
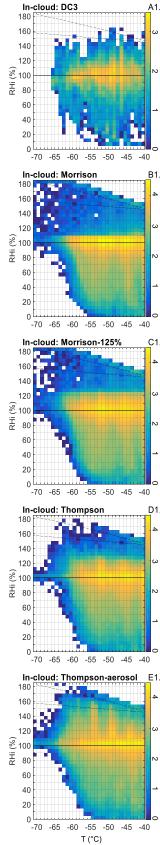
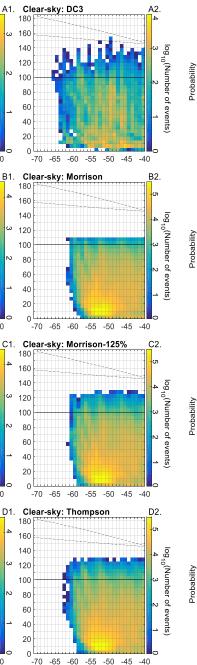
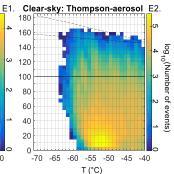


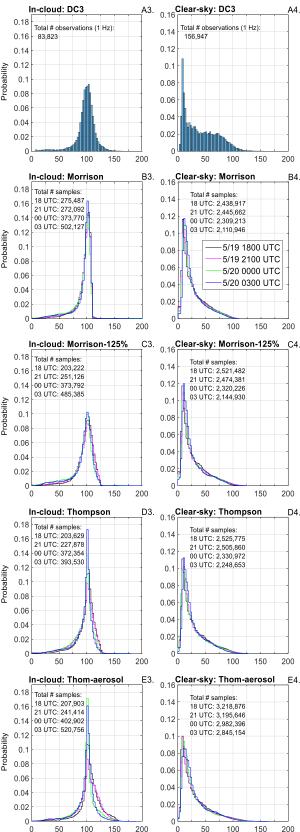
Figure 1: (A) The parent and nested domains for WRF simulations with all flight tracks from
 DC3 (thin orange lines). Distributions of RHi and vertical velocity in a horizontal cross section at

300 hPa (B) and in a vertical cross section at 40°N latitude (C and D), based on Thompson with the 2.4 km nested domain on May 20th, 2012 at UTC 0000. The May 19<sup>th</sup> flight track (thick orange line) is shown in Figure 1 B. Gray contours show RHi gradient, with shaded gray colors representing ice supersaturated regions. Vertical velocity contours are shown for -0.5 m s<sup>-1</sup> (blue), +0.5 m s<sup>-1</sup> (red), and ±5 m s<sup>-1</sup> (green). The dashed and dot-dashed lines are the 0°C and -40°C isotherms, respectively.









Α4

200

200

200

200

200

RHi (%)

E4.

D4.

B4.

797

RHi (%)

798 Figure 2: Occurrences of RHi with respect to temperature (two columns on the left) and probability density functions (PDFs) of RHi (two columns on the right) for DC3, Morrison, 799 800 Morrison-125%, Thompson, and Thompson-aerosol. The comparisons for in-cloud and clear-sky conditions are shown separately. The RHi – T distributions are based on the composite of four 801 time outputs from WRF simulations, with RHi and T binned by 5% and 1 K, respectively. The 802 PDFs of RHi show these four WRF time outputs individually in different colored lines, with RHi 803 binned by 2.5%. A total of 22 flights from DC3 are used in all the observation analysis. In the 804 RHi – T distributions, the solid and dashed lines represent the saturations with respect to ice and 805 with respect to liquid water calculated based on Murphy and Koop [2005], respectively. The 806 homogeneous freezing line (dot-dashed) is based on Koop et al. [2000] with deliquesced 807 particles at the diameters of 0.5 µm. 808

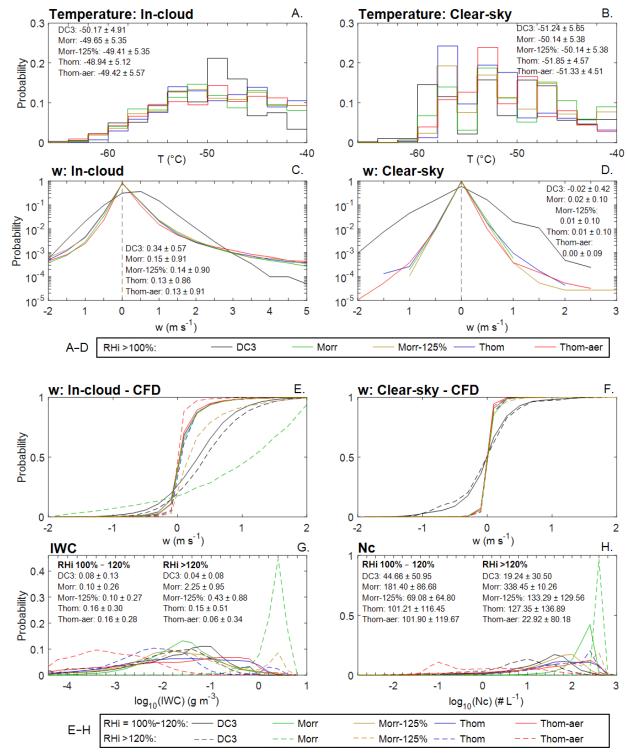
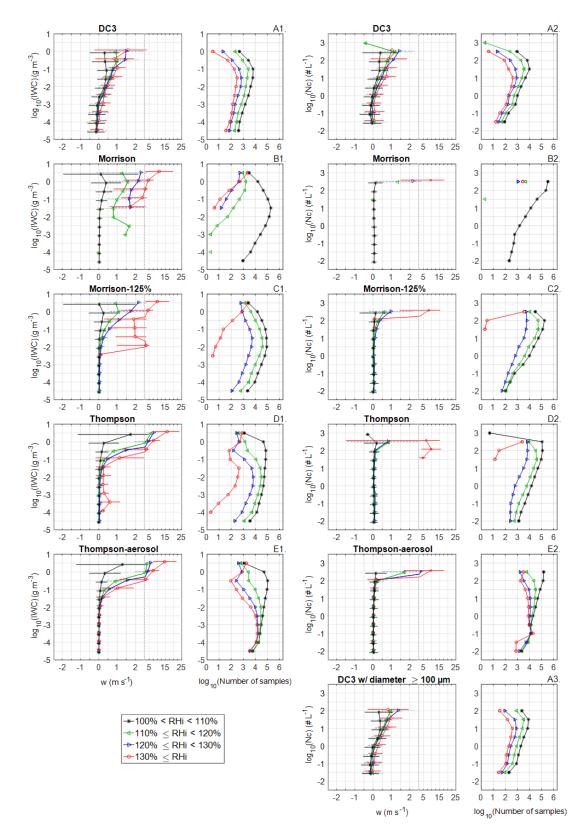




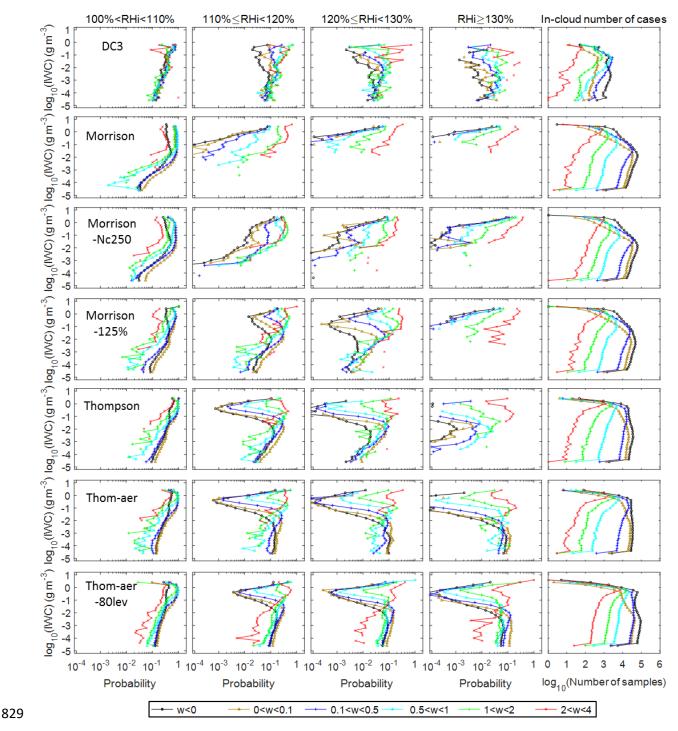
Figure 3: Normalized frequency distributions of temperature, w, IWC, and Nc for various ranges
of ISS. Distributions of temperature and w are provided for in-cloud and clear-sky conditions
(A–D). Cumulative Frequency Distributions (CFDs) of w are also provided for in-cloud and
clear-sky conditions (E & F). Normalized frequency distributions of temperature, IWC, Nc, and

- 814 w are binned by  $2^{\circ}$ C, 0.2 g m<sup>-3</sup>, 0.2 L<sup>-1</sup>, and 0.5 m s<sup>-1</sup>, respectively. The CFDs of w are restricted
- to  $\pm 2 \text{ m s}^{-1}$  and are binned by 0.2 m s<sup>-1</sup>. In A D, solid color lines represent RHi > 100% for
- various datasets. In E H, solid and dashed lines represent RHi = 100% 120% and RHi >
- 817 120%, respectively. The mean and standard deviation  $(\pm \sigma)$  of each variable are provided in their
- 818 respective figures. We note that the means and standard deviations for in-cloud and clear-sky w
- 819 are calculated over the entire distribution of their respective datasets.

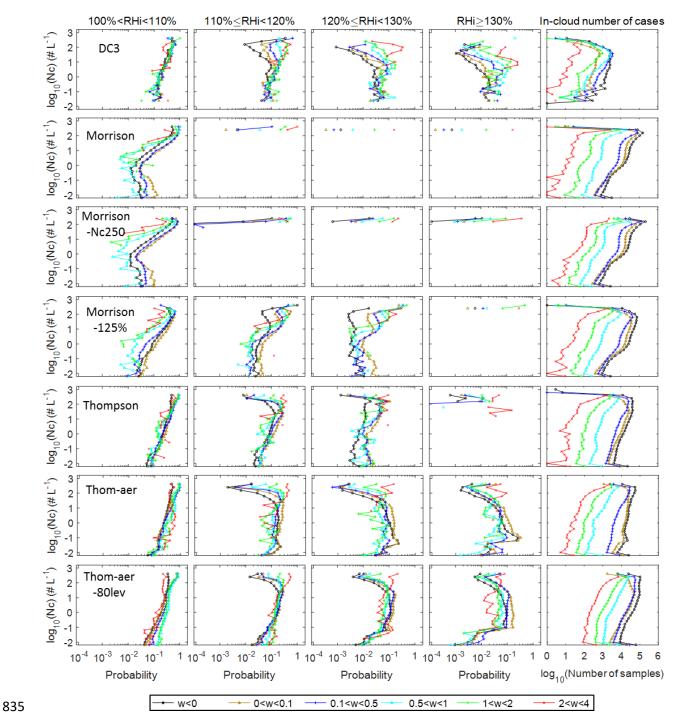


**Figure 4**: Average vertical velocity (w) binned by IWC (left two columns) and Nc (right two columns) for different ranges of ISS. Four ranges of ISS are shown in different colored lines. We

- 823 note that in order to show the different color lines clearly, we slightly shifted them vertically
- from each other, even though they are binned into the same ranges of IWC and Nc. Horizontal
- lines represent  $\pm 1 \sigma$  of the w in each bin, and the gray dashed lines highlight various ranges of w.
- 826 The total number of samples is shown in the second and fourth columns. To illustrate the
- 827 relatively small impacts from potential ice particle shattering in measurements, results with Nc
- 828 observations excluding smaller ice particles (< 100  $\mu$ m) are also shown in panel A3.



**Figure 5**: Probabilities of different magnitudes of ISS occurring at various ranges of w (shown in different colored lines), controlling for the IWC on the y-axis. The probability of a given range of ISS occurring is determined by normalizing the number of ISS occurrences in a certain ISS interval at a given range of w and IWC with the total number of occurrences of all RHi at that same range of w and IWC. Probabilities of ISS are shown in the logarithmic scale.



**Figure 6**: Similar to Figure 5, but controlling for Nc when analyzing the probabilities of different magnitudes of ISS occurring at various ranges of w. The factor of Nc is controlled on the y-axis.

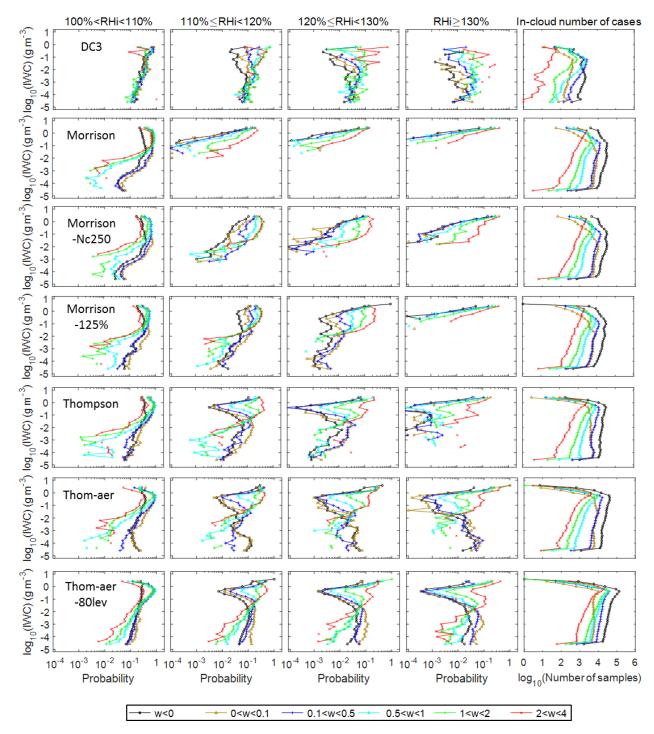
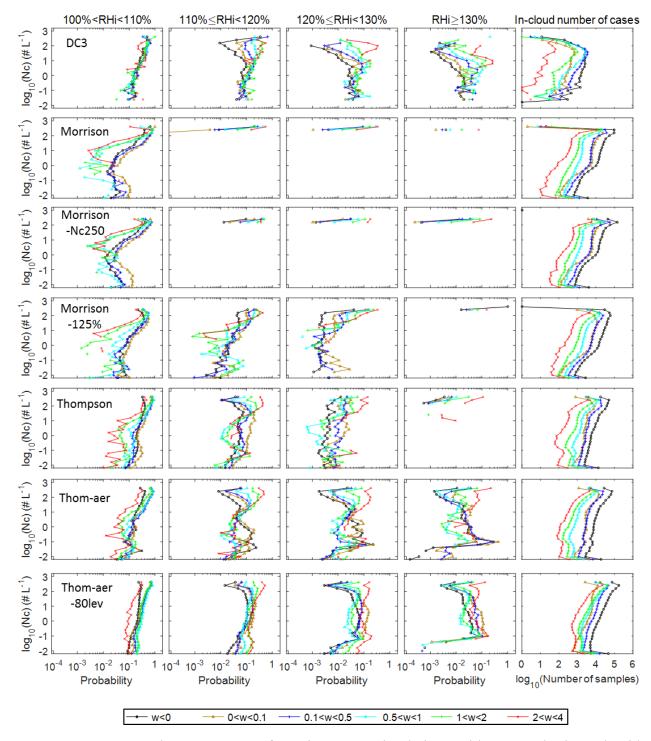


Figure 7: Same as Figure 5, except for using gridded data in a nested domain from higher
resolution WRF simulations, i.e., at 800 m horizontal grid spacing. In this figure, the WRF
datasets consist of gridded data from one time output: 20 May 2012 at UTC 0000.



**Figure 8**: Same as Figure 6, except for using WRF simulations with 800 m horizontal grid spacing. In this figure, the WRF datasets consist of gridded data from one time output: 20 May

845 2012 at UTC 0000.

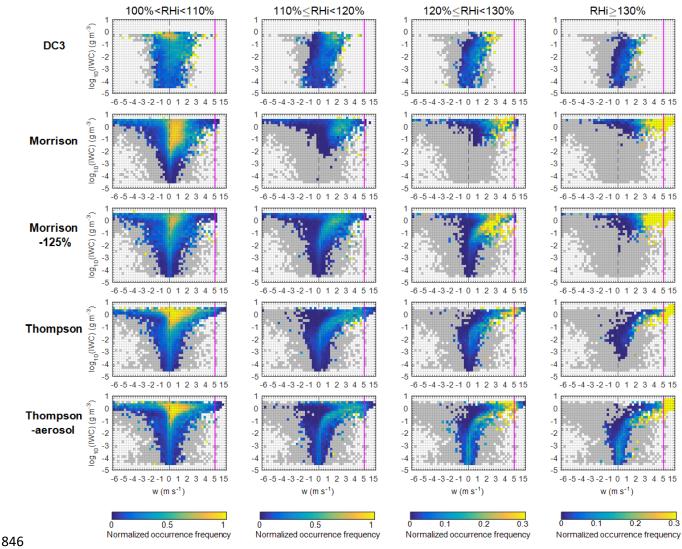
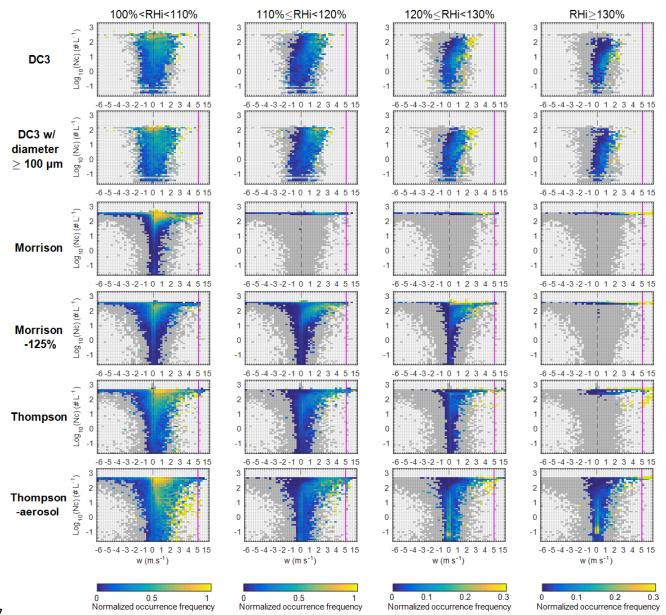


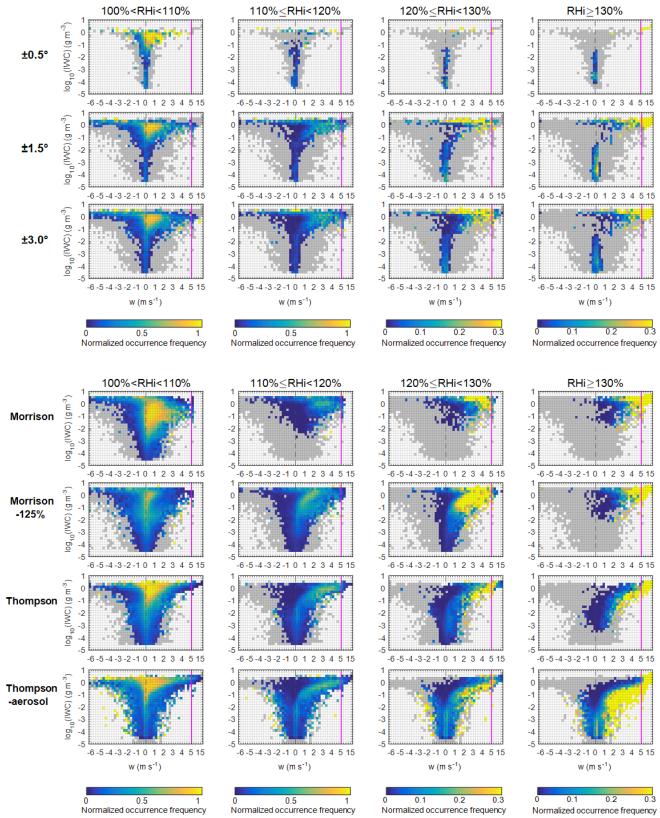
Figure 9: Normalized occurrence frequencies of ISS in relation to various magnitudes of w,

847 controlling for IWC on the y-axis. The four columns show analyses at four different ISS 848 intervals. Occurrence frequencies of ISS are calculated by normalizing the ISS occurrences at 849 each w and IWC bin with the total number of occurrences of all RHi in that bin. We note that 850 two different bin sizes of w are used here: w is binned by 0.25 m s<sup>-1</sup> for w < 5 m s<sup>-1</sup>, and by 2.5 851 m s<sup>-1</sup> for w > 5 m s<sup>-1</sup> (the maroon line highlights the transition between the two bin sizes). When 852 w is below -6 m s<sup>-1</sup> or greater than 15 m s<sup>-1</sup>, these strong downdrafts/updrafts are grouped into 853 the minimum and maximum w bins, respectively. The dashed line differentiates between 854 updrafts and downdrafts. Gray colors represent the background of all RHi being observed or 855 simulated. 856

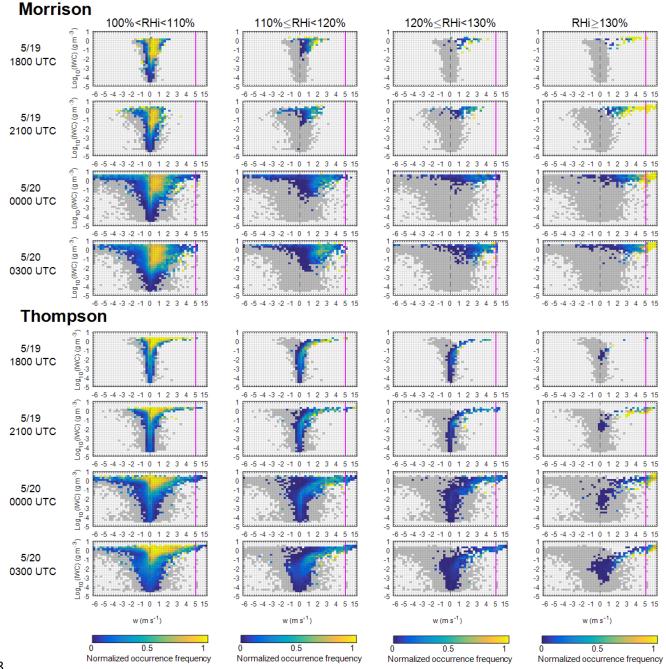


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Figure 10: Same as Figure 9, except controlling for Nc when analyzing the correlations between ISS occurrence frequencies and w. To limit the potential ice shattering effects on the in-situ measurements, results that exclude ice particles smaller than 100  $\mu$ m in DC3 dataset are shown in the second row.



**Figure 11**: Similar to Figure 9, except for (top 3 rows) gridded data from Thompson-aerosol collocated with the May 19<sup>th</sup> GV aircraft observations within  $\pm 0.5^{\circ}$ ,  $\pm 1.5^{\circ}$  and  $\pm 3.0^{\circ}$  in latitude and longitude and within  $\pm 30$  min; (bottom 4 rows) a different time period, i.e., during 11–12 June 2012 consisting of three merged time outputs (UTC 1600, 2000, and 0000).



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**Figure 12**: Similar to Figure 9, but shows four individual time outputs of WRF simulations at

- 870 UTC 1800, 2100, 0000, 0300 during 19–20 May 2012. Results of the Morrison and Thompson
- simulations are shown in the top and bottom panels, respectively.