The Importance of the Ice-Phase Microphysics Parameterization for Simulating the Effects of Changes to CCN Concentrations in Deep Convection

CAROLINE JOUAN AND JASON A. MILBRANDT

Meteorological Research Division, Environment and Climate Change Canada, Montreal, Quebec, Canada

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ABSTRACT

Simulations of a well-observed squall line that occurred during the Midlatitude Continental Convective Clouds Experiment (MC3E) were conducted using a mesoscale model with a horizontal grid spacing of 1 km to examine the importance of parameterized ice-phase processes to changes in concentrations of activated cloud condensation nuclei (CCN) in a detailed two-moment bulk microphysics scheme. Numerical experiments showed that the simulated squall-line structure was sensitive to changes in activated CCN concentration not only from the direct impacts on cloud droplet sizes and autoconversion rates, but also because of changes in the growth rates and spatial distribution of ice-phase condensate. A microphysical budget analysis highlighted the importance of graupel in rain production and the sensitivity of graupel growth rates on changes to CCN concentrations. Sensitivity tests on the level of detail in the representation of graupel, specifically the treatment of its bulk density and the number of prognostic moments, indicated that changes in the reflectivity and precipitation structure of the simulated storm due to changes in CCN were sensitive to the graupel parameterization. The results suggest that the proper representation of graupel and possibly other ice-phase categories in microphysics schemes may be crucial for correctly simulating the effects of changes to CCN concentrations for continental deep convective systems.

1. Introduction

Natural and anthropogenic atmospheric aerosols affect Earth's climate by modifying its energy balance and clouds. Recent studies show increasingly the importance of taking into account the aerosol–cloud–precipitation interactions in high-resolution (i.e., 1–3-km horizontal grid spacing) numerical weather prediction (NWP) models for improving short-term forecast accuracy, especially for mixed-phase mesoscale convective systems (MCSs; e.g., Noppel et al. 2010; Seifert et al. 2012; Thompson and Eidhammer 2014). While results from these studies showed no statically significant aerosol effect on area-averaged surface precipitation, large impacts on precipitation amounts occur locally and on in-cloud properties (Nesbitt et al. 2006). Common in both midlatitude and tropical environments, MCSs are significant rain-producing weather systems (Fritsch et al. 1986). They are organized

ensembles of convective elements whose appearance and behavior are determined by several factors, including the cold pool strength, vertical shear, ambient instability, and storm-relative winds (e.g., Houze 1993). A large number of numerical modeling studies have investigated the aerosol–cloud–precipitation interactions on mixed-phase MCSs, leading to the conclusion that the discrepancies in the results on precipitation response to aerosol loading depend not only on the MCS type and environmental factors (e.g., Tao et al. 2007; Lee et al. 2008; Khain et al. 2008; Fan et al. 2009; Storer et al. 2010; van den Heever et al. 2011; Lebo and Morrison 2014; Saleeby et al. 2016; Marinescu et al. 2017), but also on the particular model configuration and microphysics parameterization used (Lebo and Seinfeld 2011; Tao et al. 2012). Besides the accumulated surface precipitation, many weather forecast-related applications require a good representation of water-/ice-phase contents as well as their size distributions (which ultimately depend on aerosol characteristics) in order to predict, for example, in-flight aircraft icing (Thompson et al. 2017), visibility conditions of heavy-fog events (Gultepe and Milbrandt 2010), and formation and distinction between freezing rain and freezing drizzle (Stewart et al. 2015). Detailed

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Corresponding author: Dr. Caroline Jouan, caroline.jouan@canada.ca

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examination of how the upper-level cloud microphysical properties and processes, including ice phase, are ultimately affected by a change in aerosols thus becomes relevant.

With the improvements to high-performance computing, operational weather centers are moving toward kilometer-scale NWP systems, where it becomes valid and beneficial to use more detailed and realistic physics parameterizations such as for precipitation, cloud, and aerosol processes. This includes the use of detailed bulk microphysics schemes (BMSs). For example, the “aerosol aware” quasi-two-moment¹ microphysical scheme (Thompson and Eidhammer 2014) was implemented into the operational 3-km High-Resolution Rapid Refresh (HRRR; Pinto et al. 2015) prediction system from the National Oceanic and Atmospheric Administration (NOAA) and the Liquid Ice Multiple Aerosols (LIMA) quasi-two-moment microphysical scheme was implemented into the Mesoscale Nonhydrostatic (MesoNH) cloud-resolving mesoscale model from Météo-France (Vié et al. 2016). The two-moment Milbrandt and Yau (2005a,b; hereafter MY05a,b) microphysics scheme [referred to as two-moment Milbrandt–Yau (MY2)] is used in the operational 2.5-km High Resolution Deterministic Prediction System (HRDPS; Milbrandt et al. 2016) in Environment and Climate Change Canada (ECCC).

While BMSs may not be able to model the complete detailed effects of cloud–aerosol interactions, two-moment schemes are able to simulate the warm-phase coalescence process reasonably well and to capture the effects of cloud condensation nuclei (CCN) concentrations, at least to the extent that they affect the size distribution of cloud droplets (Cohard and Pinty 2000). While the effects of CCN on modeled precipitation for liquid-only cases are well understood, essentially high CCN concentrations lead to more numerous and thus smaller cloud droplets, which delays autoconversion and the onset of precipitation (Twomey 1977; Albrecht 1989; Saleeby et al. 2010), the less direct impact on precipitation response to aerosol loading due to the effects on ice-phase microphysics is less clear and there have been discrepancies in the modeling results (e.g., Noppel et al. 2010; Seifert et al. 2012; Tao et al. 2012; Fan et al. 2013; Loftus and Cotton 2014). Recent work have suggested that including the effects of CCN concentrations in bulk schemes may be sensitive to details in the parameterization of the ice-phase categories themselves, such as for the treatment of graupel density (e.g., Milbrandt and

Morrison 2013). Since BMSs are used in research to examine CCN concentration sensitivity (e.g., Storer et al. 2010; Lebo and Morrison 2014; Kalina et al. 2014; Saleeby et al. 2016) and in operational NWP (Noppel et al. 2010; Seifert et al. 2012; Thompson and Eidhammer 2014; Vié et al. 2016), it continues to be relevant to examine and discuss the effects of the representation of aerosols in atmospheric models using bulk schemes. The purpose of this study, therefore, is to examine the importance of some specific details of the parameterization of ice-phase microphysics, in particular, the representation of graupel, in a two-moment BMS to changes to CCN concentrations. The hypothesis tested is that in order to simulate correctly the effects of CCN, which directly affect cloud droplet number concentration only, the simulation of deep convective systems, as well as its sensitivity to aerosol loading, may ultimately depend greatly on details in the representation of ice.

The remainder of this article is organized as follows. Section 2 provides a description of the study case and the model configuration. Section 3 presents a validation of the control simulation. Section 4 shows sensitivity to specific ice-phase microphysical processes for extreme values of activated CCN number concentration in MY2, including microphysical budget studies. Sensitivity to graupel parameterization complexity implemented in MY2 for extreme activated CCN is discussed in section 5. A summary is given in the section 6.

2. Experimental design

a. Case overview

The 20 May 2011 squall line was the most intense MCS that occurred during the Midlatitude Continental Convective Clouds Experiment (MC3E; Tao et al. 2013; Lang et al. 2014; Fan et al. 2015; Jensen et al. 2016; Marinescu et al. 2016; Saleeby et al. 2016; Tao et al. 2016; Fan et al. 2017). In the early morning of 20 May, a strong quasi-linear MCS quickly developed into a long leading convective line with a large trailing stratiform precipitation region. Extending to approximately 1000 km, it propagated in an eastward direction across northern Texas, Oklahoma, and southern Kansas to reach its peak in size and intensity near 1100 UTC. The mature phase of the squall line lasted until approximately 1400 UTC and started to dissipate afterward (Marinescu et al. 2016; Fan et al. 2017). Saleeby et al. (2016) presented a time series of CCN number concentration from 22 to 24 May 2011 during MC3E. Concentrations were measured at the surface at various supersaturations, at the Southern Great Plains (SGP) site of the U.S. Department of

¹ Both the Thompson–Eidhammer and LIMA schemes have a two-moment treatment of cloud, rain, and ice but one-moment treatment of snow and graupel/hail.

Energy's Atmospheric Radiation Measurement (ARM) program (ARM-SGP). These results showed that the number concentration of activated CCN N_{act} varied between 600 and 2000 cm^{-3} at the highest measured supersaturations (0.85% and 1.08%, respectively), with some peaks at 4000 cm^{-3} , at the ARM-SGP site.

b. Model configuration

1) GEM MODEL AND SETUP

High-resolution 3D simulations were performed using the nested limited-area Global Environmental Multiscale (GEM) model (Côté et al. 1998; Girard et al. 2014) based on the configuration of ECCO's 2.5-km NWP system, the HRDPS over the central United States and southern Great Plains with one-way nested domains (D1 and D2) with horizontal grid spacing of 2.5 and 1 km, respectively (Fig. 1). The model uses 62 vertical sigma–pressure hybrid coordinate levels, with the lowest thermodynamic level at ~ 20 m AGL and the top at 10 hPa, described by Girard et al. (2014). The GEM model configuration details are summarized in Table 1. Simulations for domain D1 used initial and lateral boundary conditions provided by the operational 10-km Regional Deterministic Prediction System (RDPS; Mailhot et al. 2006), which covers most of the North America, every 6 h; simulations for domain D2 used initial and lateral boundary conditions obtained from domain D1 every 1 h.

2) OVERVIEW OF MY2

Cloud microphysical processes are parameterized by the MY2 bulk scheme (MY05a,b). MY2 predicts the mass contents and number concentrations for six hydrometeor categories: cloud water, rain, cloud ice, snow, graupel, and hail. The particle size distribution of each category is represented by a complete gamma function with a fixed spectral shape parameter of 1 for cloud water and 0 for rain and all ice categories. The prognostic variables are related through numerous microphysical processes whose prognostic equations [(A1)–(A7)] are described in the appendix. A complete description of the original scheme can be found in MY05a,b with modifications for the prognostic graupel density found in Milbrandt and Morrison (2013). The parameterization of CCN activation is based on Cohard and Pinty (2000). The number of activated CCN is computed from a polynomial approximation of the hypergeometric function proposed in Cohard et al. (1998) for a given environmental temperature, pressure, and vertical velocity and according to assumed total particle number concentrations of condensation nuclei for either maritime ($N_{\text{ccn}} = 66.6 \text{ cm}^{-3}$) or continental ($N_{\text{ccn}} = 842 \text{ cm}^{-3}$) air masses.

FIG. 1. GEM nested grids with domain 1 (D1) and 2 (D2) at horizontal grid spacings of 2.5 and 1 km, respectively. Analysis for D2 are presented.

c. Simulations description

All simulations are initialized at 0000 UTC 20 May 2011 and integrated for 18 h in order to encompass the development, mature, and dissipation phases of the squall line. A control simulation, described below, is first run to establish the overall fidelity of the model setup used in this study. Several sensitivity tests were then conducted. Table 2 provides the list of simulations that will be presented; the details are discussed in the following corresponding sections. The first pair of runs prescribes a low and a high activated CCN concentration. The subsequent simulations were then run in order, first, to identify the main microphysical processes that result in the differences between the low and high CCN runs, and, second, to examine the sensitivity to the level of detail in the ice-phase parameterization on the responses to changes in CCN.

3. Overview of control simulation

A control simulation (CTL; see Table 2), with the CCN specified as continental for the activation parameterization, was run in order to establish that the squall-line system is sufficiently well simulated with GEM. Figure 2 shows radar reflectivity at approximately 1 km above ground level (AGL) for the observations and from the model (CTL) at 1100 UTC when the squall line was in its mature phase (Tao et al. 2013). Radar reflectivity observations come from the National Severe Storms Laboratory (NSSL) 3D mosaic Next Generation

TABLE 1. Summary of GEM model configuration.

Model aspect	Details
Grid	Arakawa C grid (Mesinger and Arakawa 1976) Two nested horizontal grids (grid 1: 1080×984 points, $\Delta x = 2.5$ km, $\Delta t = 60$ s; grid 2: 1125×810 points, $\Delta x = 1$ km, $\Delta t = 20$ s) Vertical grid: 62 vertical levels, staggered (Girard et al. 2014), with the lowest thermodynamic level at ~ 20 m AGL and the top at 10 hPa.
Initial and lateral boundary conditions	RDPS (GEM, 10 km) + Canadian Land Data Analysis Assimilation (CaLDAS; Carrera et al. 2015)
Microphysics scheme	Milbrandt–Yau two-moment scheme (MY05a,b; Milbrandt and Morrison 2013)
Convective scheme	Kuo transient shallow convection scheme (Bélair et al. 2005)
Planetary boundary layer scheme	TKE with statistical representation of subgrid-scale cloudiness (MoistKE; Bélair et al. 2005)
Radiation scheme	Li–Barker correlated- k distribution radiative transfer scheme (called every 15 min; Li and Barker 2005)
Surface scheme	Soil, Biosphere, and Atmosphere (ISBA) land surface scheme (Noilhan and Planton 1989; Bélair et al. 2003)

Weather Radar (NEXRAD). The radar mosaic data have a 1-km horizontal resolution, a varying vertical resolution (from 200 to 2000 m), and a 5-min temporal resolution (Zhang et al. 2005). The computation of model equivalent reflectivity in MY2 is described in Milbrandt et al. (2008). Results shown in Fig. 2b illustrate that the GEM simulation correctly developed an elongated leading convective line oriented from southwest to northeast with a bowing structure, as observed (Fig. 2a). Behind the leading convective line, the simulation also captures a large trailing stratiform region. However, the weak echo transition zone, due to subsidence and suppression of precipitation particle growth (Braun and Houze 1994), which is clearly evident in observations between the convective line and the trailing stratiform region, is not well captured in the GEM simulation, which produces a wider area of high reflectivity greater than 45 dBZ in the convective region. This exaggeration of the width of the convective regions is consistent with a known bias of MY2 (Morrison et al. 2015; Fan et al. 2017).

Figure 3 shows the time series of 1-h accumulated precipitation from CTL and observations. Precipitation observations come from two products. The first is the NEXRAD National Mosaic and Multisensor Quantitative

Precipitation Estimate (QPE) product (NMQ Q2) with a rain gauge adjustment (Q2_GAUGE). Q2_GAUGE data are provided with a 1-km horizontal spacing and a 1-h frequency (Zhang et al. 2011). The second is the National Centers for Environmental Prediction stage IV QPE (Q2_STAGEIV) using both radar and gauge data to produce quantitative precipitation amounts with 4-km horizontal spacing and 1-h frequency (<https://doi.org/10.5065/D6PG1QDD>; Lin 2011). The adjusted Q2_GAUGE precipitation amounts have higher values than the surface rain gauge network (Oklahoma Mesonet observations; Brock et al. 1995), while the Q2_STAGEIV agreed much better with the Oklahoma Mesonet observations (J. Wang 2016, personal communication). Results from Fig. 3 show that the simulated and observed systems developed at the same time, with a rapid increase of precipitation starting at 0600 UTC. Considering that the Q2_GAUGE tend to represent the higher end of observed precipitation values, MY2 likely overestimates the accumulated precipitation in the D2 analysis domain.

Despite some shortcomings, the CTL simulation reproduced the main observed features of the squall line, including time and space evolution, precipitation, and radar reflectivity with sufficient accuracy for the

TABLE 2. List of simulations and their modifications in MY2.

Runs	Details
CTL	Original MY2 with background CCN concentration in continental mode and fixed graupel density ρ_g
CLN	As CTL, but with the <i>clean</i> activated CCN concentration ($N_{\text{act}} = 100 \text{ cm}^{-3}$)
POL	As CTL, but with the <i>polluted</i> activated CCN concentration ($N_{\text{act}} = 4000 \text{ cm}^{-3}$)
CLN_2A	As CLN, but with no autoconversion process
CLN_2B	As CLN_2A, but with a lower graupel collection efficiency E_{cg} [D_{mc} in (4) is replaced by D'_c , which use a fixed $N'_{ic} = N_{\text{act}} = 4000 \text{ cm}^{-3}$]
CLN_3A	As CLN, but with prognostic ρ_g
POL_3A	As POL, but with prognostic ρ_g
CLN_3B	As CLN, but with one moment for graupel
POL_3B	As POL, but with one moment for graupel

FIG. 2. (a) NEXRAD reflectivity and (b) CTL simulated reflectivity at 1 km AGL for the 20 May 2011 event at 1100 UTC.

purposes of this study. Simulation of this case using the setup of CTL with the MY2 scheme can therefore be used for the following sensitivity experiments to investigate the sensitivity of the ice-phase parameterization to changes in CCN.

4. Sensitivity of ice-phase processes to CCN concentrations

In the following tests, the effects of increasing the CCN number concentration has been simplified by removing the parameterization of aerosol activation and prescribing directly the number concentrations of activated CCN (i.e., newly formed cloud droplets) N_{act} as either $N_{\text{act}} = 100 \text{ cm}^{-3}$, representative of a very clean, or $N_{\text{act}} = 4000 \text{ cm}^{-3}$, representative of highly polluted continental environments. The N_{act} is initialized at these values everywhere for a given simulation and does not vary in time or space. This is a simplification of the activation process, but it is acceptable for this study whose objective is to examine the impacts of the ice-phase parameterization to the responses of changes to CCN concentrations. The increase in CCN number concentration in nature generally leads to the increase of activated CCN number concentrations, which is controlled by the peak supersaturation, and typically occurs just above cloud base. The cloud droplets number concentration for nonprecipitating clouds is thus determined at this level, above which it has an approximately constant value (e.g., see Rogers and Yau 1989, their Fig. 7.4). In MY2, the cloud nucleation rate is calculated from the maximum of the existing total number concentration of cloud droplets and the number concentration of nearly

activated CCN where there is supersaturation. Then changes to the mass content and total number concentration of cloud droplets are predicted to evolve because of other microphysical processes.

The lowest prescribed N_{act} is chosen to be lower than what is typically obtained with the assumed background continental CCN concentration as in the CTL simulation. The highest prescribed N_{act} is chosen on the basis of the peak values observed in Saleeby et al. (2016) at supersaturation of 1.08%. These two CCN sensitivity runs are denoted CLN and POL for the low and high N_{act} values, respectively (Table 2). Relatively extreme N_{act} values are chosen in order to clearly identify changes to

FIG. 3. Time series of hourly accumulated precipitation, averaged over D2, for the CTL simulation and the two observational data products (rain gauge-adjusted NEXRAD QPE denoted by “Q2_GAUGE” and the stage IV QPE denoted by “Q2_STAGEIV”) from 0100 to 1800 UTC 20 May 2011. Time series of precipitation rate for the clean conditions (CLN; solid) and polluted conditions (POL; dotted) simulations are also presented in magenta (see Table 2 for simulations description).

CLN

FIG. 4. Time evolution, from (a) 0400 to (i) 1200 UTC, of spatial distribution of reflectivity for the CLN simulation at 1 km AGL. The gray shading indicates D2. The vertical distribution of line-averaged microphysical fields in Fig. 6 (left) were calculated between the red lines in (h). The black dashed box represents the squall-line system domain used to calculate the microphysical budget in Fig. 8 (left).

the storm simulations through responses in the microphysics scheme. Note that the goal of this study is not to examine the sensitivity of squall lines to CCN per se, whose responses to changes in background CCN concentrations are nonlinear. Rather, we seek to identify specific aspects of parameterized ice-phase microphysical processes

whose details may ultimately be important in correctly simulating the effects of changes to CCN.

a. Reflectivity structure and precipitation

Figures 4 and 5 show the time evolution of the spatial distribution of model reflectivity at 1 km AGL from

POL

FIG. 5. As in Fig. 4, but for the POL simulation.

CLN and POL, respectively. In both simulations, a precipitating convective system appears after 2 h, located in the domain D2 center (Figs. 4a and 5a). A few hours later, the squall line of interest develops behind the existing precipitating convective system, with which it eventually merges after 12 h. Clear differences appear at 0800 UTC where model reflectivity is much larger in POL compared to the CLN (Figs. 4e and 5e); while in

CLN, the separation between the trailing stratiform region and the convective line is better reproduced.

The time series of 1-hourly accumulated precipitation from the CLN and POL simulations are shown in magenta in Fig. 3. In CLN, the squall line developed 1 h earlier than in POL (Figs. 4a and 5a), with a rapid increase of precipitation starting at 0500 UTC in CLN. Results from other studies also showed that high

TABLE 3. Accumulated total surface precipitation (mm) from 0600 to 1200 UTC averaged over D2 from observations and model simulations described in Table 2.

Run	Amount
Q2_GAUGE	6.72
Q2_STAGEIV	4.85
CTL	7.28
CLN	8.17
POL	6.84
CLN_2A	7.26
CLN_2B	7.01
CLN_3A	8.55
POL_3A	7.70
CLN_3B	7.62
POL_3B	7.00

concentrations of activated CCN could result in the delay of the onset of precipitation mainly because of a delay in warm-rain growth process (e.g., Albrecht 1989; Khain et al. 2005; van den Heever et al. 2006; Storer et al. 2010; Thompson and Eidhammer 2014).

During the main development phase (0600–1200 UTC) of the squall line, the hourly surface precipitation averaged over the D2 domain varies by a factor of 1.19 from the CLN and POL. This is the same order of magnitude as between CTL and observations (1.08–1.50) and between the two types of observations (1.39; Table 3). Taking into account the error in the observations, these results seem to show no significant aerosol effect on area-averaged surface precipitation. However, using high-resolution (1-km grid spacing) models simulations, Fan et al. (2017) found, for the same case, that the averaged accumulated surface precipitation, from 0600 to 1200 UTC, varied by up a factor of 1.5 from different microphysics schemes, including for the MY2. Thus, the precipitation response to aerosol loading appears to be the same order of magnitude as precipitation response for the different microphysical schemes used in that study.

b. Vertical distribution of hydrometeors characteristics

Figure 6 shows the vertical distribution of the line-averaged microphysical fields of the squall line at 1100 UTC, toward the end of its mature phase. Both simulations have a typical reflectivity structure of a characteristic leading convective zone with an extensive zone of stratiform precipitation and a well-defined melting-layer signal (see the 0°C isotherm level; dashed line; Figs. 6a,f). However, the POL reflectivity (Fig. 6f) tends to have higher values than CLN (Fig. 6a) over the entire squall line, because of larger snow mass contents in stratiform regions (Figs. 6d,i) and larger hail mass contents (Figs. 6e,j) in convective regions. In both CLN and POL simulations,

the weak echo transition zone is still not well represented.

At first glance, the results show that an increase in N_{act} leads to an increase in the mass of slow-falling hydrometeors such as the cloud water with higher values at higher mass content q_c levels in the squall-line convective region (between 32.8° and 33.2°N; Figs. 6b,g), the ice crystals q_i , and snow mass content q_s (Figs. 6d,i). Although q_c , q_i , and q_s have considerably increased, the mass content (Fig. 6e,j) of graupel q_g decreases significantly with increasing activated CCN concentration. The mass content of hail q_h slightly increases with increasing N_{act} (Fig. 6e,j). In MY2, graupel is formed mainly by collection of supercooled cloud water by snow, which is converted to graupel. When the ambient air temperature is below 0°C, rain can also freeze directly to graupel (or to hail). In CLN, graupel is transported horizontally throughout almost the entire extent of the stratiform region (latitude >33.3°N), with its contents all above or near the 0°C isotherm level (~4-km altitude; Fig. 6e). In POL, the q_g total and peak quantities tend to decrease and are shifted downward, under the 0°C isotherm level (between 32.8° and 33.3°N; Fig. 6j). This suggests that graupel grows to larger mean sizes in polluted conditions with a higher fall speeds through the updrafts, thus limiting their horizontal transport to the stratiform region and promoting the formation of larger hail (from graupel), which can sediment to lower levels before melting completely (this is shown in Fig. 9c described in the next section). The vertical distribution of rain (Figs. 6c,h) clearly shows a decrease in the rain mass content q_r in the convective region with a slight increase in the stratiform region due to CCN loading.

c. Microphysical budget study

1) MICROPHYSICAL BUDGET SETUP

To help understand the microphysical pathways within the MY2 scheme that result in the large differences noted in the spatial distribution of hydrometeors throughout the storm with different CCN concentrations, a microphysical budget analysis was conducted. The budget is calculated following the method proposed by Colle and Zeng (2004) and Colle et al. (2005) and serves to determine the relative importance of each microphysical process in transferring water mass from one category to another one. Over the entire region of the squall line, each microphysical process rate QAB_{xy} (listed and described in the appendix) is output every 10 min. Data are then averaged over a 6-h period of squall-line development phase (between 0600 and 1200 UTC) and integrated in the vertical (k) and horizontal (i, j) coordinates before being normalized by the

FIG. 6. Cross section of microphysical fields averaged perpendicularly between the two red lines in Fig. 4h for (a)–(e) CLN and Fig. 5h for (f)–(j) POL at 1100 UTC 20 May 2011. The microphysical fields represented are (a),(f) reflectivity; (b),(g) cloud water number concentration [cm^{-3} ; solid contour lines (start, step)] and cloud water mass content (g m^{-3} ; color bar); (c),(h) rain number concentration [m^{-3} ; contour solid line (start, step)] and rain mass content (g m^{-3}); (d),(i) ice cloud [contour solid line at 0.005, 0.01, 0.02, 0.03, 0.04, 0.05 g m^{-3}] and snow (color bar) mass content (g m^{-3}); and (e),(j) graupel (color bar; g m^{-3}) and hail [solid contour lines at 0.005, 0.02, 0.04, 0.06, 0.08, 0.1, 0.2 g m^{-3}] mass content. Radar reflectivity ($\text{mm}^6 \text{m}^{-3}$), mass content, and number concentration have been averaged including cloudless grid points.

FIG. 7. The result of partitioning into convective and stratiform regions in the (a) CLN and (b) POL simulations at 1100 UTC 20 May 2011.

integrated water vapor loss (WVL) within that same grid box to obtain a microphysical tendency ratio AB_{xy} :

$$AB_{xy} = \frac{\sum_{i,j,k} QAB_{xy}(i,j,k)\rho(i,j,k)}{\sum_{i,j,k} WVL(i,j,k)\rho(i,j,k)} \times 100\%, \quad (1)$$

where ρ is the air density and WVL is the water vapor loss rate defined by the sum of the sink terms in the water vapor budget:

$$WVL = QVD_{vc}[\text{condensation}] + QVD_{v,ish}[\text{deposition}] + QNU_{vi}. \quad (2)$$

The microphysical budget was first computed separately for the convective and stratiform regions of the storm, identified by the partitioning method similar to the one described in [Marinescu et al. \(2016\)](#) and [Saleeby et al. \(2016\)](#), which takes into account the precipitation rate, vertical velocity, and cloud mass content. [Figure 7](#) shows the result of partitioning method for the convective and stratiform area in CLN and POL at 1100 UTC 20 May 2011. The broader convective region in POL is evident. The microphysical budget was also computed over the entire squall line. Although there are differences in the convective and stratiform regions, the same general conclusions, regarding the relative differences in process rates, can be made from the budget over the entire storm. Thus, to simplify the discussion of the results only the budgets over the entire system are presented.

2) RELATIVE CONTRIBUTIONS OF MICROPHYSICAL PROCESSES

[Figure 8](#) summarizes the average microphysical budget over the squall line from 0600 to 1200 UTC for CLN

and POL. Data are averaged over the regions indicated by the dot-dashed rectangles in [Fig. 4](#) from CLN and [Fig. 5](#) for POL. Microphysical process values greater than 10% of the WVL rate are highlighted in bold in [Fig. 8](#).

Not surprising, the most important pathway of water vapor depletion is condensation (cond) with $VD_{vc}(\text{cond} = 78.12\%)$ of WVL in CLN and $VD_{vc}(\text{cond} = 85.83\%)$ of WVL in POL. Graupel depositional (depo) growth [$VD_{vg}(\text{depo} = 16.99\%)$] is another important pathway for water vapor depletion in CLN and deposition onto snow [$VD_{vs}(\text{depo} = 8.22\%)$] dominates in POL, mainly in stratiform region (not shown). The deposition rates are greater when the total surface area of particles population is large and the particles are numerous. [Figure 9](#) shows the mean differences in mass content, number concentration, and mean diameter of each hydrometeor between CLN and POL averaged between 0600 and 1200 UTC over the entire squall line. [Figures 9b and 9c](#) show that snow has larger number concentrations and mean sizes in POL than in CLN, which is consistent with the higher value of snow depositional growth. To explain the increase of snow content, an increase in N_{act} (POL) decreases the mean size of cloud droplets below 7-km altitude ([Fig. 9c](#)) and thus also the bulk collection efficiency (which depends on droplet sizes), reducing the accretion rate ($CL_{cr} = 16.83\%$) and the autoconversion rate ($CN_{cr} = 0.00\%$ in POL; [Fig. 8b](#)), thus suppressing the warm-rain processes. The autoconversion parameterization in MY2 is adopted from [Berry and Reinhardt \(1974\)](#) and [Cohard and Pinty \(2000\)](#) and is active when the standard deviation of the diameter of cloud droplets exceeds $15 \mu\text{m}$. In POL, the decrease of cloud droplet size due to high CCN concentration reduces the standard deviation of

FIG. 8. Microphysical flowchart for the MY2 between 0600 and 1200 UTC of the (a) CLN and (b) POL simulations. The circle represents the various categories: water vapor (w.v.), cloud water (c.w.), rain, cloud ice (c.i.), snow, graupel (grpl), and hail. The arrows are the microphysical tendencies ratio (AB_{xy}) that link the categories. The values shown are the ratio of each microphysical process rate to the total WVl rate ($VD_{wc}[cond] + VD_{v,slgh}[dep] + NU_{sl}$) within the black dashed box in [Figs. 4 and 5](#). The sum (source + sink) of all the microphysical tendencies ratio of each categories is given by w.v., c.w., r, c.i, s, g, and h notations. The sum does not include horizontal advection and diffusion. The fallout tendency of rain (Rprc), snow (Sprc), graupel (Gprc) and hail (Hprc) are also shown. Microphysical processes greater than 10% of the WVl rate are in boldface.

the distribution thereby completely shutting off auto-conversion in MY2. This suppression of warm-rain processes makes it possible to retain more q_c in the system (Fig. 9a), which is then transported vertically and freezes homogeneously to ice crystals at higher levels ($FZ_{ci} = 8.78\%$ in POL; Fig. 8b). This in turn leads to increased latent heat release and further convective invigoration (see following section). This results in an average increase in cloud ice both in number concentration

and in size below 10-km altitude (Figs. 9b,c) linked to a slight increase of cloud ice deposition (VD_{ui} is 1.81% more; Fig. 8) because of the higher total surface area of cloud ice. More snow is then formed by growth of ice crystals and then grows by deposition. Then this new amount of cloud ice aloft gets rapidly converted to snow ($CN_{is} = 12.09\%$ of WVl in POL; Fig. 8b), as shown by increasing the snow number concentration and size (Figs. 9b,c). This increase in q_s with increasing aerosols is consistent with previous model results (e.g., Li et al. 2008; Seifert et al. 2012; Storer and van den Heever 2013).

As seen in [section 4b](#), q_g is less in POL (as well as the graupel number concentration; [Figs. 9a,b](#)), limiting the growth of graupel by deposition (VD_{vg} is 16.99% in CLN and 2.63% in POL; [Fig. 8](#)). The lower graupel number concentration in POL may be attributed to the reduction of the collisional freezing rate between graupel and rain [i.e., CL_{grg} in [Figs. 8a,b](#) corresponding to $\delta_{grg}(QCL_{gr} + QCL_{rg})$ in (A6)]. The CL_{grg} is a factor of 2.76 lower in POL and mainly depends on the collection of graupel by rain value (CL_{gr}), which is much lower in CLN (16.68%) than in POL (5.49%) because of the suppression of warm-rain processes.

The lower graupel mass content in POL may be attributed to the reduction of the collisional freezing rate between graupel and rain discussed previously, associated to the graupel riming rate, which is about 20% larger in CLN than in POL ($CL_{cg} = 23.82\%$ for CLN and 19.81% for POL; Fig. 8). The rate of graupel collection of cloud droplets is computed from the stochastic collection equation (SCE; see MY05b) using a bulk collection efficiency E_{cg} that depends on the mean-mass droplet size (Cober and List 1993). While the SCE is nonlinearly related to mass content and number concentration of the hydrometeor category being collected, since the cloud droplets have such a small fall speed compared to graupel, the collection rate from the analytic solution to the SCE is very similar to that rate given by a simple continuous collection equation if both approaches assume the same E_{cg} . Given that there is more cloud water available for collection in POL (Fig. 6) yet CL_{cg} is reduced in POL, this implies that differences in graupel growth rates for different activated CCN concentrations are strongly affected by the droplet size effect because of the parameterized collection efficiency, which would have led to the large decrease of graupel in the POL simulations. This is examined further below. Note that for the same squall-line case, Saleeby et al. (2016) found an opposite effect of an increase riming of cloud droplets due to increased cloud droplets number concentration under polluted conditions.

Hail, once initiated, grows mainly via rain collection in both the CLN and POL runs before becoming an

FIG. 9. Differences (POL – CLN) in (a) mass content, (b) number concentration, and (c) mean mass diameter of each hydrometeor, averaged between 0600 and 1200 UTC 20 May 2011 over the black dashed box in Figs. 4 and 5.

important source of rain at lower levels by melting ($ML_{hr} = 32.51\%$ in CLN and 25.46% in POL; Fig. 8). The cloud water collection by hail increases (CL_{ch} of 3.19% more in POL; Fig. 8) from CLN to POL, which may explain the slight increase of hail mass content to higher altitudes (>4.5 km) in the mixed phase (Fig. 9a). It should be noted that in nature, hail is defined as high-density rimed ice that has either a graupel or frozen raindrop embryo and typically has a diameter greater than 5 mm (Young 1993). In MY2, the hail category includes all frozen raindrops, allowing the mean diameter of newly formed “hail” in MY2 to be quite small, even though it does not fit the conventional definition of natural hail. Thus, it is perfectly reasonable to have large mass contents of model hail in the stratiform region in the simulated squall line.

For rain with low N_{act} , the collection of cloud water (CL_{cr}) is the main microphysical growth process in the convective region (not shown), whereas the most relevant microphysical processes responsible for rainfall are the melting of graupel (ML_{gr}), hail (ML_{hr}), or snow (ML_{sr}) in the stratiform region (not shown). At higher N_{act} , the production of rain by warm-rain processes is of secondary importance in this case. An increase in N_{act} leads to the production of fewer but larger raindrops because of liquid-phase processes. This can be attributed to changes in cloud droplet spectra that directly impact cloud droplet self-collection and accretion, which are the main processes for generating rain at a temperature higher than 0°C . However, below this several

microphysical processes (drop self-collection, accretion of droplets, collection of rain by ice-phase hydrometeors, melting, and evaporation) interact in a net competing and nonlinear manner to impact the raindrop size. The production of fewer larger raindrops at a temperature lower than 0°C appears to scale with the production of fewer, larger graupel.

d. Impact on updraft speed

Figure 10 shows the vertical profiles of updraft velocity w averaged over the squall line for grid points with $w > 2 \text{ m s}^{-1}$ and between 0600 and 1200 UTC for various simulations (Fig. 10a) and for differences from CLN (Fig. 10b). For POL, there is increased vertical motion compared to CLN from approximately 2.5 to 7.5 km AGL, indicating a convective invigoration effect due to aerosol loading. Convective invigoration occurs as additional latent heat is released because of the freezing of more liquid water, which is retained aloft because of a less efficient warm-rain process (production of precipitation-sized drops from droplet coalescence; Andreae et al. 2004; Rosenfeld et al. 2008). However, the trend reverses in upper levels and updrafts are weaker for POL (Fig. 10b). A similar effect was noted in Storer and van den Heever (2013) for simulated tropical deep convective clouds between high and low aerosol concentrations, where it was identified that increased condensate loading above the freezing level in high aerosol cases causes a reversal in the average vertical motion trend. Also, Fan et al. (2009, 2012) noted that the

FIG. 10. Vertical profiles of updraft velocity w , averaged over the squall line for grid points with $w > 2 \text{ m s}^{-1}$ and between 0600 and 1200 UTC for (a) various simulations and (b) differences from CLN.

aerosol invigoration effect is reduced with stronger vertical wind shear, such as in the 20 May squall-line case (Fan et al. 2017).

The dynamics of the simulated storm are altered by changes to the activated CCN concentrations. Thus, the interpretation of what and how specific aspects of the microphysics parameterization cause changes to the simulations becomes somewhat complicated in the following sensitivity tests since it is impossible to separate fully the direct effects from changes to the microphysics from indirect effects due to changes in storm dynamics (and thus subsequent forcing for the microphysics). However, the changes to the vertical motion due to changes in aerosol concentrations are sufficiently small (Fig. 10) such that the investigation still allows us to identify specific aspect in the ice-phase representation that ultimately are important to simulate the responses the CCN concentrations.

e. Sensitivity experiments for specific processes

In this section, we attempt to identify the effects of CCN that are beyond simply the direct effects of autoconversion but also indirect effects of growth processes parameters of ice-phase particles. The case is rerun based on the CLN configuration for N_{act} , but with one simulation having cloud water autoconversion completely shut off (CLN_2A) and the second using, in addition, a lower bulk collection efficiency of cloud

droplets by graupel (CLN_2B). With these tests, we attempt to explain further the differences between the CLN and POL simulations and ultimately to identify and explain aspects of the ice-phase scheme that contribute to the response to changes in CCN.

1) CLOUD WATER AUTOCONVERSION

The autoconversion parameterization is strongly dependent on the mean cloud droplet size. A low- N_{act} simulation CLN_2A with no autoconversion of cloud water was run. The vertical distribution of averaged microphysical fields at 1100 UTC (Figs. 11a–e) shows an increase in q_c , q_i , and q_s when removing autoconversion compared to CLN, with similar profiles to those of POL (Figs. 6g,i). The q_s field has slightly lower amounts for CLN_2A (Fig. 11d) than that of POL (Fig. 6i). The vertical distribution of graupel and hail are close to the POL simulation because with little graupel and hail transport in to the stratiform region (Fig. 11e). However, q_g remains high compared to POL (Fig. 6j). The vertical distribution of graupel in CLN_2A is still quite different from CLN and POL (Figs. 6e,j) with high values at q_g in the convective core but lower values in the stratiform region. For the vertical distribution of rain (Fig. 11c), when removing the autoconversion, the stratiform rainfall increases whereas the convective rainfall slightly decreases, as in POL (Fig. 6h).

FIG. 11. As in Fig. 6, but for (a)–(e) CLN_2A and (f)–(j) CLN_2B, averaged over similar regions as in Fig. 5h, but relative to the CLN_2A and CLN_2B storms, respectively.

To isolate the effects of activated CCN concentrations on the simulated storm due only to the parameterized collection efficiency between cloud water and graupel, another sensitivity test CLN_2B was run, following from CLN_2A (with low N_{act} and autoconversion off), but now the value of the mean-mass cloud diameter D'_{mg} used in (4) to compute E_{cg} is computed using the predicted value of q_c but a fixed value of $N_c = 4000 \text{ cm}^{-3}$, equivalent to N_{act} in POL, rather than the predicted N_c , which is strongly dependent on the low N_{act} . All other appearances of D_{mc} in the scheme use the normal D_{mc} value computed from q_c and the predicted N_c .

The vertical distribution of averaged microphysical fields for CLN_2B at 1100 UTC is shown in Figs. 11f–i. CLN_2A and CLN_2B have similar q_c fields (Figs. 11b,g) since they have the same N_{act} and autoconversion setting. However, since the mean-mass droplet diameter used to compute E_{cg} is smaller in CLN_2B than in CLN_2A, the collection efficiencies are lower in CLN_2B [see (4)] and thus so are the graupel riming rates, $Q_{CL_{cg}}$. By reducing E_{cg} , the amount of snow, q_s , is increased, since more q_c “escapes” being collected by graupel in CLN_2B and is thus transported to higher levels in the convective regions, where it then freezes homogeneously to ice, some of which is then later converted to snow. In contrast, q_g and q_r decrease in CLN_2B, especially in the convective region. This brings the CLN_2B simulation even closer to POL. The microphysical budget of CLN_2B (not shown) indicates that the process rates for CLN_2B are very similar to those of POL (Fig. 8b). The effects of the collection efficiency between hail and cloud water E_{ch} on the riming rates of hail were not tested, but E_{ch} is parameterized based on Ziegler (1985) and also depends on D_{mc} , implying the activated CCN concentration also impacts the riming rate of hail.

The two sensitivity experiments discussed above allow us to account for a majority of the large differences between the simulated squall lines in CLN and POL. Certainly just shutting off autoconversion in the low-CCN configuration (or in effect, computing autoconversion based on high N_{act}) accounts for many of the differences, since the CLN_2A simulation is more similar to POL than to CLN. This is not surprising; however, the direct effect of N_{act} on the warm-phase coalescence process does not account for all the notable differences. The effects on the mean cloud droplet size on the riming rates of ice-phase categories, in particular graupel, due to the changes in the bulk collection efficiencies have a notable impact on the values and spatial distribution of frozen condensate and thus ultimately on the reflectivity and precipitation structures of the simulated storm.

It is reasonable to expect, therefore, that the response to changes in CCN in simulated deep convective systems

will be sensitive in general to parameterized ice-phase processes that have a dependency on the cloud droplet number concentration and/or the mean droplet diameter. By implication, if the ice-phase processes in the microphysics scheme being used are not parameterized with the correct dependency on cloud droplet size and number, the simulated responses to aerosols will not be completely correct, regardless of the complexity and accuracy of aerosol and liquid-phase components of the scheme.

5. Sensitivity of the parameterization of graupel to CCN

The sensitivity experiments discussed above indicate the importance of parameterized ice-phase processes for correctly simulating the impacts of aerosols on deep convective systems. This section examines further the impact of the level of complexity in the parameterization of graupel in modeling the effects of changes to CCN concentrations. Specifically, we investigate the sensitivity to the treatment of the bulk graupel density ρ_g and the number of prognostic moments by conducting four additional simulations with the prescribed low and high N_{act} but with a prognostic ρ_g configuration (CLN_3A and POL_3A) and a one-moment graupel configuration (CLN_3B and POL_3B).

a. Prognostic graupel density

In all of the simulation discussed so far, ρ_g had a fixed value of 400 kg m^{-3} and fixed parameters for the fall speed–diameter relation, as in the original MY2 code. Milbrandt and Morrison (2013) described a development to the scheme in which the ρ_g is prognostic, using a rime density parameterization based on laboratory experiments, and graupel fall speeds are computed consistently, based on the density and size. In an idealized kinematic framework, they illustrated that CCN concentration ultimately affects the rime density and thus ultimately impacts the simulation of graupel and rain. In the context of this current study, therefore, two simulations were conducted, with the prescribed low and high N_{act} values but now with prognostic ρ_g . The runs are denoted CLN_3A and POL_3A.

The vertical distribution of the line-averaged microphysical fields at 1100 UTC for these simulations is shown in Fig. 13 (see Fig. 14 and the discussion in section 5b for CLN_3B and POL_3B). The microphysical fields between CLN (Figs. 6b–e) and CLN_3A have similar profiles except for a slightly smaller graupel content for CLN_3A. However, the two simulations POL

FIG. 13. As in Fig. 6, but for (a)–(e) CLN_3A and (f)–(j) POL_3A, averaged over similar regions as in Figs. 4h and 5h, but relative to the CLN_3A and POL_3A storms, respectively.

FIG. 14. As in Fig. 6, but for (a)–(e) CLN_3B and (f)–(j) POL_3B, averaged over similar regions as in Fig. 5h but relative to the CLN_3B and POL_3B storms, respectively.

FIG. 15. Differences in mass content between (a) POL and CLN, (b) POL_3A and CLN_3A, and (c) POL_3B and CLN_3B of each hydrometeor, averaged between 0600 and 1200 UTC 20 May 2011 over the black dashed box drawn in Figs. 4 and 5.

(Figs. 6h,i,j) and POL_3A (Figs. 13h,i,j) have notably different profiles of ice, snow, and graupel. Figure 12b summarizes the average microphysical budget over the storm for POL_3A. The results show that the high N_{act} in POL_3A leads to a suppression of autoconversion and a reduction of the cloud collection rate ($\text{CL}_{\text{cr}} = 17.50\%$) with the same order of magnitude as in POL (Fig. 8b) with fixed ρ_g . This results in retaining more q_c , which subsequently freezes homogeneously ($\text{FZ}_{\text{ci}} = 3.44\%$) and is converted to snow ($\text{CN}_{\text{is}} = 6.34\%$); however, the process rates have about half of the values in POL, even though the two simulations have the same initial N_{act} . This reduction in the magnitude of the homogeneous freezing rate and rate of conversion from cloud ice into snow (CN_{is}) is consistent with the higher collection rate of cloud water by the graupel ($\text{CL}_{\text{cg}} = 27.30\%$) compared to POL. As discussed in Milbrandt and Morrison (2013), since the inclusion of a prognostic ρ_g leads to larger ρ_g because of larger instantaneous rime density, the effects of the sizes of droplets/drops being collected are accounted for.

In principle, we would expect a better simulation of a deep convective storm with a better representation of rimed ice. However, the important point in the context of this study is that with the inclusion of the prognostic graupel density (and a more realistic effect on graupel fall speeds) in the squall-line simulations, the response to the CCN loading between CLN_3A and POL_3A is quantitatively different in terms of magnitudes compared to the response in CLN and POL, though qualitatively similar in terms of structure and distribution. Figure 15 shows the mean differences in mass content of

each hydrometeor between CLN and POL and between CLN_3A and POL_3A, averaged between 0600 and 1200 UTC. An increase in N_{act} has less impact on the mass of ice-phase hydrometeors (ice, snow, graupel, and hail) for the prognostic- ρ_g configuration (Fig. 15b) than for the fixed- ρ_g configuration (Fig. 15a).

The different responses to CCN loading may be attributed to the microphysical responses to the prognostic ρ_g . By comparing the averaged updraft velocity during 0600–1200 UTC between CLN-POL and CLN_3A-POL_3A in Fig. 16b, it is shown that the switch to prognostic ρ_g has similar impact on the updraft velocity of the squall line. Figure 17 shows the time series of hourly precipitation difference for CLN-POL, CLN_3A-POL_3A, and CLN_3B-POL_3B. The most significant feature is that an increase in N_{act} generally increases the accumulated precipitation (Table 3) for most simulations, except at the time of the squall-line maturation phase for the last two simulations (Fig. 17). The CCN effect on precipitation appears to be more significant at the dissipation stage with prognostic ρ_g compared to fixed ρ_g . However, the changes to this aspect of the treatment of graupel do not change the sensitivity to CCN concentration qualitatively.

The differences in precipitation distribution when changing the level of sophistication of ice-phase scheme can be attributed to the fact that the most relevant microphysical processes responsible for the rainfall are the melting of graupel and hail (Figs. 8 and 12) associated with the fact that the relationship between enhanced-CCN effects and precipitation are nonlinear. Thus, the CCN effect on precipitation changes depends also on the

FIG. 16. As in Fig. 10, but with simulations CLN and POL (magenta), CLN_3A and POL_3A (blue), and CLN_3B and POL_3B (green).

treatment of ρ_g in the microphysics scheme. This adds support to the conclusion of the previous section: if the parameterized ice-phase processes lack realism, such as a realistic representation of graupel density and its correct impact on terminal fall speed, the simulated responses to CCN loading for simulated deep convective storms may be incorrect.

b. One moment for graupel

It is well recognized that the two-moment bulk approach for parameterizing cloud microphysics is generally superior to the one-moment approach, particularly for the modeling of deep convective storms (e.g., Swann 1998; Milbrandt and Yau 2006; Morrison et al. 2009; Dawson et al. 2010; Van Weverberg et al. 2012; Igel et al. 2015; Loftus and Cotton 2014; Morrison et al. 2015; Dodson et al. 2018). However, it is not necessarily obvious that the two-moment representation of ice-phase categories would be particularly important in order to simulate the correct overall response to CCN loading for droplet nucleation. Therefore, following the arguments in the previous section, another set of low and high N_{act} sensitivity simulations was run, this time with the graupel category (only) set to one moment. That is, MY2 was set to have a prognostic graupel mass content but with the intercept parameter of the size distribution fixed at $4 \times 10^6 \text{ m}^{-4}$ (and thus a diagnostic number concentration),

as in the one-moment configuration tested in Milbrandt and Yau (2006). These runs are denoted CLN_3B and POL_3B (Table 2); all other configuration aspects (including fixed ρ_g) are identical to CLN and POL.

The results for CLN_3B and POL_3B are shown in Fig. 14. Comparison of the vertical distribution of

FIG. 17. Time series of hourly precipitation differences between CLN and POL (magenta), CLN_3A and POL_3A (blue), and CLN_3B and POL_3B (green) from 0600 to 1200 UTC 20 May 2011.

microphysical fields between simulations POL (Figs. 6g–j) and POL_3B show similar profiles at 1100 UTC. However, the two simulations, CLN and CLN_3B, show different profiles of cloud droplets number concentrations and snow and graupel mass contents (Figs. 6b,d,e and Figs. 14b,d,e). Despite a low N_{act} , CLN_3B exhibits a higher snow mass content than CLN, and the graupel is limited in its horizontal transport into the stratiform region.

The effects on hydrometeor sedimentation from two moment to one moment (see MY05a) slightly changed the vertical redistribution of q_g , N_{Tg} (the total number concentration of graupel), and D_{mg} . With a two-moment scheme, q sediments at a faster bulk fall velocity than N_T , allowing a realistic size-sorting effect, whereby D_m is redistributed in the vertical with larger (smaller) D_m appearing at relatively lower (higher) levels. In a one-moment scheme, N_T and D_m are diagnosed directly from q with a single mean fall speed for particles of different sizes, resulting in vertical profiles of q , N_T , and D_m being therefore similar (e.g., MY05a). The graupel growth rates are thus much different with a one-moment treatment. Ultimately, this results in a much different vertical and thus horizontal distribution of graupel mass, which is particularly evident in comparison of CLN (Fig. 6e) and CLN_3B (Fig. 14e). However, to have a vertical and horizontal distribution of the graupel sensitive to N_{act} , this suggests that the BMS must be at least two moment for graupel. Figure 12c summarizes the average microphysical budget from 0600 to 1200 UTC for experiment CLN_3B. The results indicate that more cloud droplets (higher N_c) arrive at higher levels (Fig. 14b) that are then frozen to cloud ice and converted into snow ($FZ_{ci} = 2.63\%$; $CN_{is} = 4.73\%$) than in CLN (Fig. 8a). The homogeneous freezing rate is quite sensitive to act as trigger for the production of snow mass to the detriment of graupel mass content.

Overall, except for the expected impact on auto-conversion and cloud water mass, an increase in N_{act} has little impact on the mass of ice-phase hydrometeors (ice, snow, graupel, and hail) for the one-moment graupel configuration (Fig. 15c). This includes the effect on the hourly precipitation whose differences CLN_3B–POL_3B is smaller than CLN–POL over the entire period of development of the squall line (Fig. 17). Thus, the sensitivity experiments show that with the one-moment graupel configuration, the response to CCN loading is much less sensitive than with the two-moment graupel configuration. Again, the implication is that in order to simulate the effects of CCN loading correctly, the level of complexity (realism) in the parameterization of the ice phase is important, particularly the representation of rimed ice (graupel/hail).

6. Summary and discussion

There have been conflicting results in previous modeling studies regarding the impacts of CCN concentration on deep convective systems using cloud-resolving model simulations. This appears to be due in part to indirect effects related to the parameterization of ice microphysics. This study was conducted to examine the level of detail of the ice-phase component of a detailed bulk microphysics scheme that is necessary to simulate the responses to changes in CCN concentrations with fidelity. To that end, a midlatitude continental squall line that was well observed during the MC3E experiment was simulated with a mesoscale model using a fully two-moment bulk scheme. Various sensitivity experiments were conducted in which elements of the graupel parameterization were modified for various pairs of simulations with high and low concentrations of activated CCN. Examination of reflectivity structures, hydrometeors distributions, precipitation, and microphysical budgets indicated that the representation of graupel in particular plays a key role for determining the response of the simulated storm to changes in CCN.

Since the CCN concentration affects the cloud droplet number concentration and hence the mean droplet diameter, the microphysical response of the model depends on the extent to which the parameterized processes involving the ice phase realistically account for the effects of droplet sizes. In the MY2 scheme, used in this study, the mean droplet size affects graupel growth directly through the collection efficiency between graupel and droplets and, in the prognostic graupel density configuration, through the instantaneous rime density. Sensitivity tests showed that changes to the representation of these aspects changed the response in the simulated storm to modifying the activated CCN concentration. It was also shown that whether the graupel category is one moment or two moment also has a notable impact on the response to CCN. Thus, changes to the level of detail in the parameterized ice microphysics, in particular for graupel, have a significant impact on the responses to changes in CCN concentrations for a simulated deep convective system, at least for the case tested. If it did not, the changes to the reflectivity structure, hydrometeor mass distribution, and precipitation due to changes in CCN concentration between each pair of simulations with different N_{act} would be the same regardless of the details of the representation of graupel.

Interpretation becomes complicated by the fact in some simulations changes to CCN result in changes to the microphysical process rates, which cause changes to

the storm dynamics, which in turn feed back to the microphysics. The piggyback method (Grabowski 2014, 2015) would make it possible to confidently assess the relative impacts of the microphysics versus the dynamics. However, the goal of this study was to investigate the extent to which the parameterized ice-phase microphysics ultimately matters for correctly simulating the CCN effects. Regardless of the relative direct contributions from dynamical and/or microphysical effects, it can certainly be concluded that if modifying an aspect of the ice-phase component of the microphysics schemes changes the simulated responses to CCN concentration changes, then clearly, the details of that aspect of the parameterization must be important to simulate correctly the effects of aerosols in the model. Here, we have identified the correct representation of graupel in the microphysics scheme as being important.

Some limitations of this study are worth noting, though they do not weaken the conclusions significantly. First, constant values—uniform at all levels—of activated CCN concentration [i.e., cloud droplet number concentration (upon nucleation)] are prescribed in our simulations. This simplification is acceptable for the purposes of this study since cloud droplet number concentration (before autoconversion, etc.) is determined just above cloud base, where the peak supersaturation is normally reached. However, several studies showed that the nonhomogeneous CCN distribution (in addition to ice nuclei and giant CCNs), and the chemistry of CCN needs to be considered to assess the aerosol–cloud–precipitation interactions (e.g., Ekman et al. 2004, 2006; Levin et al. 2005; Tao et al. 2012; Fan et al. 2018). In the same way, the simplification of the aerosol process treatments, such as wet/dry scavenging and the aerosol activation, can lead to unrealistic estimates of their number concentration and properties leading to an overestimation or underestimation of their potential impact in cloud microphysical processes. Second, only one autoconversion parameterization (Berry and Reinhardt 1974) was used. It is possible that the simulated responses to CCN concentration changes may be different with different autoconversion schemes. However, this is not likely to interfere with the interpretation of the effects of the representation of the ice phase. Third, while we make the argument regarding the importance of the correct representation of graupel, the MY2 scheme does have some known weaknesses in the graupel category. Collection between rain and graupel is parameterized with an analytic solution to the stochastic collection equation, which is problematic for collection between categories with similar fall speeds such as rain and graupel. A better approach is to compute the collection rates in bin space and create lookup tables, such

as is done in Saleeby and Cotton (2008), Thompson and Eidhammer (2014), and Morrison and Milbrandt (2015). Thus, the prognostic graupel density full two-moment MY2 configuration may not necessarily be the best possible bulk representation of graupel. Nevertheless, the conclusions regarding the graupel–cloud droplet collection efficiency, treatment of graupel density, and the need for at least two-moment graupel should still be valid regardless at any differences in MY2. Also, the effects of three-moment graupel were not considered in this study. Based on the results of Milbrandt and Yau (2006), however, the changes in the simulation between three-moment and two-moment graupel should be much smaller than the changes between two moment and one moment; therefore, although three moment is generally preferable, the two-moment treatment of graupel is probably sufficient in that regard to capture the effects to CCN changes.

Although this study dealt with a single case and used a single microphysics scheme, it is reasonable to expect this conclusion would be true for other deep convective systems and for other schemes. At the very least, modelers should be cautious of the representation of graupel in the microphysics scheme. The implication of the conclusions argued is that if, for a given atmospheric modeling application that attempts to capture the effects of CCN—either for process studies or for NWP—if the microphysics scheme lacks sufficient realism in the representation of rimed ice, then the accuracy of the model response to changes in the background CCN concentrations may be in question. It should be noted that the argument regarding the importance of the representation of graupel is equally valid for bin microphysics schemes as for bulk schemes. The realism in bin schemes for the modeling of droplet activation, the liquid-phase coalescence process, and hydrometeor size distributions increases in general. However, if the scheme lacks a realistic treatment of rime density and/or has arbitrary thresholds for the conversion from one ice-phase category to another, then the simulated effects of CCN on deep convective systems should be questioned. Thresholds for the conversion from one ice-phase category to another are an inherent and unphysical necessity for any scheme, bin or bulk, that partitions ice into predefined categories.

Motivated from the budget studies, the focus in the sensitivity tests conducted was on graupel. There are other ice-phase processes in microphysical schemes that also depend on mean droplet sizes, including the riming rates of snow and hail and the conversion rates for snow to graupel and for graupel to hail, all of whose

parameterization details may affect the response to the incorporation of aerosols for CCN. One aspect of the graupel category in all traditional category-based schemes, such as MY2, is that the simulation of graupel (and other ice-phase categories) is very sensitive to arbitrary thresholds for the artificial processes of conversion between categories. As a closing comment, we remark that the sensitivity to ice-phase representation discussed in this study lends support to the general idea advocated by Morrison and Milbrandt (2015; and others) of abandoning the use of predefined ice-phase categories in microphysics schemes and moving toward particle property-based approaches for the representation of ice in models. Ultimately, improving the representation of rimed ice in microphysics schemes should, among other benefits, lead to more accurate simulations of the effects of aerosols in models.

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APPENDIX

MY2 Bulk Scheme Prognostic Equations

In MY2 scheme mass mixing ratio (kg kg^{-1}) of water vapor q_v , cloud water q_c , cloud ice q_i , rain q_r , snow q_s , graupel q_g , and hail q_h are related through

a numerous microphysical processes and described in the following prognostic equations [(A1)–(A7); MY05b]:

$$\frac{dq_v}{dt} = -QVD_{vc} - QVD_{vr} - QNU_{vi} - QVD_{vi} - QVD_{vs} - QVD_{vg} - QVD_{vh}, \quad (\text{A1})$$

$$\frac{dq_c}{dt} = QVD_{vc} - QCN_{cr} - QCL_{cr} - QFZ_{ci} - QCL_{cs} - QCL_{cg} - QCL_{ch}, \quad (\text{A2})$$

$$\begin{aligned} \frac{dq_r}{dt} = & QCN_{cr} + QCL_{cr} + QVD_{vr} + QML_{ir} + QML_{sr} \\ & + QML_{gr} + QML_{hr} - QCL_{ri} - QCL_{rs} \\ & - QCL_{rg} - QCL_{rh} + QSH_{hr} - QFZ_{rh}, \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \frac{dq_i}{dt} = & QNU_{vi} + QFZ_{ci} + QVD_{vi} + QIM_{si} + QIM_{gi} \\ & - QCL_{ir} - QCL_{is} - QCL_{ig} - QCL_{ih} \\ & - QCN_{is} - QML_{ir}, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} \frac{dq_s}{dt} = & \delta_{srs}(QCL_{rs} + QCL_{sr}) + QCN_{is} + QVD_{vs} \\ & + QCL_{cs} + QCL_{is} - QCN_{sg} - QCL_{sr} \\ & - QCL_{sh} - QIM_{si} - QML_{sr}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} \frac{dq_g}{dt} = & \delta_{irg}(QCL_{ir} + QCL_{ri}) + \delta_{srg}(QCL_{sr} + QCL_{rs}) + \delta_{grg}(QCL_{gr} + QCL_{rg}) + QCN_{sg} \\ & + QCL_{cg} + QCL_{ig} - QCL_{gr} + QVD_{vg} - QCN_{gh} - QML_{gr} - QIM_{gi}, \end{aligned} \quad (\text{A6})$$

$$\begin{aligned} \frac{dq_h}{dt} = & \delta_{irh}(QCL_{ir} + QCL_{ri}) + \delta_{srh}(QCL_{sr} + QCL_{rs}) + \delta_{grh}(QCL_{gr} + QCL_{rg}) + QFZ_{rh} \\ & + QCN_{gh} + QCL_{ch} + QCL_{rh} - QSH_{hr} + QCL_{ih} + QCL_{sh} + QVD_{vh} - QML_{hr}. \end{aligned} \quad (\text{A7})$$

The microphysical process rate ($\text{kg kg}^{-1} \text{s}^{-1}$) is denoted by QAB_{xy} , where Q represents the mixing ratio prognostic variable, AB is the microphysical process (CL for collection, CN for conversion, FZ for freezing, IM for ice multiplication, ML for melting, NU for nucleation, SH for shedding, and VD for diffusional growth), and the subscript xy indicates the transfer of mass from species category x to y (for $x, y \in [v, c, r, i, s, g, h]$). The

δxyz correspond to the delta function for the three-component freezing between hydrometeors category x and y to produce category z .

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