Diagnosing the Intercept Parameters of the Exponential Drop Size Distributions in a Single-Moment Microphysics Scheme and Impact on Supercell Storm Simulations

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Abstract

In this study, power-law relations are developed between the intercept parameter $N_0$ of the exponential particle size distribution and the water content for the rain, hail, graupel and snow hydrometeor categories within the Milbrandt and Yau microphysics scheme. Simulations of the 3 May 1999 Oklahoma tornadic supercell are performed using the diagnostic relations for rain only, and alternately for all four precipitating species, and results are compared with those from the original fixed-$N_0$ single- and double-moment versions of the scheme. Diagnosing $N_0$ for rain is found to improve the results of the simulation in terms of reproducing the key features of the double-moment simulation while still retaining the computational efficiency of a single-moment scheme. Results more consistent with the double-moment scheme are seen in general storm structure, cold pool structure and intensity, and the number concentration fields. Diagnosing the intercept parameters for all four species, including those for the ice species, within the single-moment scheme yields even closer agreement with the double-moment simulation results. The decreased cold pool intensity is very similar to that produced by the double-moment simulation, as is the areal extent of the simulated storm. The diagnostic relations are also tested on a simulated squall line, with similar promising results. This study suggests that compared with traditional fixed intercept parameters used in typical single-moment microphysics schemes, results closer to a double-moment scheme can be obtained through the use of diagnostic relations for the parameters of the particle size distribution, with little extra computational cost.
1. Introduction

As numerical weather prediction (NWP) models gain convection-resolving grid spacings of 1 km or less, the parameterization of microphysical processes becomes critical. Generally, bulk microphysics (MP) parameterizations, which specify a particular size distribution for each hydrometeor species and predict certain moments of the size distribution (e.g., the water mass, proportional to the third moment of the size distribution), are used due to the comparatively high cost of non-bulk spectral or bin models for simulations of three-dimensional moist convection.

The most commonly used particle size distribution (hereafter PSD) for precipitating hydrometeors is the inverse exponential distribution, which can be written as

\[ N(D) = N_0 \exp(-AD), \]

where \( N_0 \) is the intercept parameter and \( A \) is the slope parameter of the PSD. Usually \( N_0 \) is assigned a fixed value for each category in single-moment (SM) MP schemes. The most well-known of these exponential distributions is the Marshall-Palmer (Marshall and Palmer 1948) distribution, which specifies the rain intercept parameter \( N_{0r} \) to be \( 8 \times 10^6 \) \( \text{m}^{-4} \). However, using this fixed value for \( N_{0r} \) has been shown to be restrictive, as \( N_{0r} \) can vary significantly within single precipitation events both spatially and temporally (Tokay and Short 1996; Zhang et al. 2008; Waldvogel 1974). Snook and Xue (2008) investigated the effect of varying \( N_0 \) for the rain and hail PSDs on storm evolution within high-resolution supercell simulations, focusing on the effect upon tornadogenesis. It was found that in simulations where \( N_0 \) was lowered such that the PSD favored large drops or hailstones, the resulting cold pools were weaker and the simulations tended to develop into single or multiple supercells, while when \( N_0 \) was increased, the storms transformed to a linear mode during the simulations. Tornado-like low-level vortices formed in the low-\( N_0 \) simulations but not in others. Cohen and McCaul (2006) performed simulations using
an increased median volume diameter for hail and graupel, equivalent to decreasing the \( N_0 \) value for those species, which resulted in reduced low-level cooling due to decreased melting. Earlier studies of van den Heever and Cotton (2004) and Gilmore et al. (2004) also found significant sensitivity of simulated supercell storms to PSD parameters. More recently, Morrison et al. (2009), Dawson et al. (2010, hereafter DXMY10), and Yussouf et al. (2013) compared SM and double-moment (DM) MP schemes for simulations of squall lines and supercells, respectively (DXMY10 also considered a triple-moment scheme), likewise finding large sensitivity to the number of moments predicted, with the DM schemes typically performing better than their SM counterparts. Van Weverberg et al. (2011) investigated the impact of PSD assumptions in a SM MP scheme on precipitation and storm dynamics, and the sensitivity of a simulated squall line to two-moment MP complexity (Van Weverberg et al. 2012).

The distribution represented by (1) is a special case of the gamma distribution (Ulbrich 1983), which has the form

\[
N(D) = N_0 D^\alpha \exp(-\Lambda D),
\]

(2)

where \( \alpha \) is the shape parameter, a dimensionless measure of the spectral width of the distribution. If \( \alpha \) is set to 0, the distribution is reduced to the inverse exponential form. The addition of the shape parameter allows the gamma distribution to depict a far greater range of PSDs than the inverse exponential distribution. Mallet and Barthes (2009) applied a maximum likelihood technique to categorize rain drop size distributions (DSDs) from optical disdrometer data, and found that 91% of the measured DSDs were of the gamma type.

The values of the gamma distribution parameters vary widely in nature, both between and within a given precipitation event: thus parameterizing any of them as constant will introduce a source of error into the MP. Ulbrich (1983) calculated a typical range of values for \( \alpha \) and \( N_0 \) of
the rain DSD, encompassing relations derived from Z-R (reflectivity-rain rate) relationships presented in a number of other studies. Calculated values for $\alpha$ varied from -3.42 to 5.04 (the range was far narrower for studies based on convective rain, with $\alpha$ ranging from 0.40 to 1.63) and values for $N_0$ ranged from $1.29 \times 10^3 \text{ m}^{-4}$ to $9.20 \times 10^{12} \text{ m}^{-4}$ ($7.05 \times 10^6 \text{ m}^{-4}$ to $2.46 \times 10^8 \text{ m}^{-4}$ for convective rain). Although some of the variations in parameter values are due to errors in measurements, modeling, and fitting procedures (Cao and Zhang 2009), variation due to physical causes appears to dominate (Zhang et al. 2003; Milbrandt and Yau 2005a;b, hereafter MY05a,b respectively).

The role of the shape parameter $\alpha$ was investigated in detail by MY05a, who showed that the rate of gravitational particle size sorting was dependent on $\alpha$, with the size sorting rate decreasing as $\alpha$ increases and approaching 1 as $\alpha$ becomes large. Size sorting is an intrinsic process within supercell evolution, as witnessed by the occurrence of the differential reflectivity ($Z_{\text{DR}}$) arc within supercells (Kumjian and Ryzhkov, 2008). Hence it is important to parameterize the PSD in a realistic manner, allowing all parameters to vary as appropriate.

Thus, one way to improve a MP scheme is to increase the number of predicted moments of the PSD (Straka and Mansell 2005; MY05a). How the moments of the PSD are calculated depends on the way the PSD is parameterized. For the gamma distribution the $n^{\text{th}}$ moment is calculated as

$$M_n = N_0 \Lambda^{-(\alpha+n+1)} \Gamma(\alpha+n+1). \quad (3)$$

Most bulk MP schemes only predict one moment of the distribution, typically the third moment, $M_3$, which is proportional to the hydrometeor mixing ratio, $q$. In this case, it is usually the slope parameter $\Lambda$ that is effectively prognostic while $N_0$ and $\alpha$ are held constant. More recently, MP schemes that predict two or more moments have become increasingly popular,
particularly for convective scale modeling. Most of the DM schemes available predict both $q$ and
$N_0$, leaving $\alpha$ held constant while $N_0$ and $\Lambda$ are directly linked to the predicted variables (e.g.,
MY05b; Morrison et al. 2005).

More recently, data assimilation methods have been employed for PSD parameter
estimation, and to test the sensitivity of model outputs such as precipitation to the value of
certain PSD parameters. Tong and Xue (2008a,b) used an ensemble Kalman filter for
simultaneous estimation of the model state and MP parameters including $N_0$ for rain, snow, and
hail. Model output state sensitivity to PSD parameter values has been investigated using a
Markov chain Monte Carlo algorithm to produce joint probability density functions of the model
output state and PSD parameters (Posselt and Vuki
cevic 2010). The joint PDFs for model output
state and $N_0$ for snow and graupel ($N_{0s}$ and $N_{0g}$) were shown to exhibit multimodality, due to a
transition from convective to stratiform precipitation (Posselt and Bishop 2012). The transition
from convective to stratiform precipitation has also been shown to alter the joint PDFs for MP
processes such as evaporation and $N_0$ of rain, snow, and graupel (van Lier-Walqui et al. 2012).
This further illustrates that using a single fixed value for $N_0$ for all types of simulation is not
appropriate. As an alternative way of addressing microphysics uncertainties, van Lier-Walqui et
al. (2014) proposed to estimate uncertain factors multiplying various microphysical process rate
terms in microphysics parameterization schemes, using an ensemble Kalman filter.

Aside from moving to multi-moment schemes, which are computationally expensive,
other methods of extending low-moment schemes beyond the fixed single-parameter approach
have been attempted. The most common method relates a free parameter in the PSD to another
independently predicted PSD parameter. Zhang et al. (2001) investigated relations between the
PSD parameters using video disdrometer data collected in Florida and derived a relation between
the shape and slope parameters. The $\alpha - \Lambda$ relation was subsequently updated using disdrometer measurements for rain DSDs observed in Oklahoma (Cao et al. 2008).

Zhang et al. (2008) used the same disdrometer data as Cao and Zhang (2009), gathered in central Oklahoma during the summers of 2005 through 2007, to derive a relationship between $N_0$ of the inverse exponential PSD and the rain water content $W_r$ (which, like mixing ratio $q_r$, is proportional to the third moment of the distribution). The diagnostic relation was formed using the method of moment relations, outlined in detail in their paper. Their derived relation for rain was $N_{0r}(M_2, M_4) = 7106 \ W_r^{0.648}$, where $N_{0r}$ is measured in $\text{# m}^{-3} \text{mm}^{-1}$ and $W_r$ is in $\text{g m}^{-3}$. Here $N_{0r}$ is given as a function of $M_2$ and $M_4$ because its relation is derived from these two moments.

In the SM version of the Milbrandt and Yau (hereafter, MY) MP scheme (MY05b), described in more detail in section 3, the PSD of each precipitating hydrometeor category is modeled by a gamma distribution with a fixed value of $\alpha$. In this paper, we assume $\alpha$ to be zero, leading to the exponential distribution commonly used in SM and DM schemes.

Given the moment relation in (3) and setting $\alpha$ to zero, we see that the exponential PSD parameters, $N_0$ and $\Lambda$, can be determined using any two moments of the distribution. Given any two moments, $M_j$ and $M_k$, the PSD parameters can be calculated as

$$N_0 = \frac{M_j \Lambda^{j+1}}{\Gamma(j+1)},$$

$$\Lambda = \left[ \frac{M_j \Gamma(k+1)}{M_k \Gamma(j+1)} \right]^{\frac{1}{k-j}}.$$

The moment estimates from disdrometer measurements contain errors (Zhang et al. 2008), causing errors in the DSD parameters determined from them. The middle (second and fourth) moments were used in their study as they contain the least error (Cao and Zhang 2009).
The main issue with these observation-based studies is that the diagnostic relations are derived using disdrometer data collected at the surface, primarily for rain. Aircraft observational campaigns have also provided information on the drop size distributions of rain (e.g., Beard et al 1986, Yuter and Houze 1997), snow (e.g., Houze et al. 1979, Field et al. 2005) and ice (e.g., Heymsfield et al. 2006).

Diagnostic relations derived from three-dimensional data sets for individual species are needed for use within MP parameterization schemes.

The goal of this study is to formulate and test diagnostic relationships between $N_0$ and $W$ for each precipitating hydrometeor species, and implement this within the SM MY MP scheme (MY05b) available within the ARPS model (Xue et al. 2000, 2001). It is hypothesized that this should allow a more realistic PSD model than the use of a fixed value of $N_0$ for each precipitating hydrometeor species, and will enable a more accurate representation of the PSDs. To this end, the overall aim of the study is to bring the results of the SM MP scheme more in line with the results of the corresponding DM MP scheme. For the derivation of the PSD parameter relationships in this study, the zeroth and third moments of the inverse exponential PSD are used since these are independently predicted within the DM MY MP scheme. As the first proof-of-concept attempt and because of the general lack of DSD observations for multiple species in 3D volumes, we use the output of the MY DM simulation to derive the relations. We leave to future work an investigation of the representativeness of surface DSDs relative to those aloft for the purpose of formulating diagnostic relations.

The remainder of the paper is organized as follows: the case being simulated is described in section 2. The formulation of the diagnostic-$N_0$ relationships is covered in section 3. The setup
used for the numerical experiments is described in section 4. Section 5 includes results of the experiments and discussion. Section 6 summarizes the results and discusses future work.

2. The May 3rd 1999 Oklahoma tornadic supercell case

On May 3rd 1999, one of the most significant tornado outbreaks ever to occur in the U.S. caused extensive damage across Oklahoma and Kansas, including the metropolitan areas of Oklahoma City and Wichita. Fifty eight tornadoes struck within the county warning area of the Norman, Oklahoma National Weather Service Forecasting Office over a period of eight hours (Speheger et al. 2002). Sixteen of these tornadoes were rated F2 or greater on the Fujita (1971) scale, including two F4 and one F5 tornadoes. The F5 tornado tracked through the small community of Bridge Creek, parts of Moore, southern Oklahoma City, Del City and Midwest City, causing 36 direct fatalities (Brooks and Doswell 2002) and injuring 583 people.

Observations from the Oklahoma Mesonet (Brock et al. 1995) and mobile mesonets (Markowski 2002) indicated that the cold pools associated with the tornadic supercells in central Oklahoma were mainly small and relatively weak. The synoptic setup for the event exhibited a large-scale trough located over the Western United States, with an embedded short-wave trough over Arizona. The large-scale trough amplified as it passed over the Rockies, and the short-wave trough propagated over western Oklahoma and Kansas, while a deepening surface low was located over the central high plains (Thompson and Edwards 2000). The low-level flow was south-to-southeast over the southern Great Plains. More detail on the synoptic setup for the event can be found in Thompson and Edwards (2000) and Roebber et al. (2002).

Given the inherent instability present, a gap in the cirrus cloud cover allowed a cumulus tower to develop close to Lawton in southwestern Oklahoma, around 2030-2045 UTC. This evolved into the first supercell and after an initial split, rapidly developed into a right-moving
supercell – storm A (Thompson and Edwards 2000). Storm A became tornadic and produced at least fourteen distinct documented tornadoes between 2151 UTC on May 3 and 0125 UTC on May 4 (Speheger et al. 2002). The most intense of the tornadoes produced by storm A was A9, the F5 tornado that left a 37-mile trail of destruction through the communities of Bridge Creek, Moore and Oklahoma City. DXMY10 simulated a supercell storm within an environment believed to be representative of the environment that storm A developed, and the study found substantial sensitivity of the simulated supercell storm to the number of moments predicted with versions of the MY scheme. Their predicted cold pool was generally too strong when using a single moment scheme while that predicted using a three-moment scheme was found to be the best.

3. Diagnostic relations for $N_0$

As pointed out previously, DSD observations for multiple species in 3D volumes are generally unavailable, making it difficult to obtain diagnostic relations for several species that are applicable to the entire storm. As the first proof-of-concept attempt, we use the output of a DM simulation for the 3 May 1999 case to derive diagnostic relations for use in a SM scheme. This allows us to see how close the results of a SM scheme with diagnostic relations can be to those of a DM scheme.

Using a single sounding to define the storm environment, DXMY10 have shown that, for the 3 May 1999 case, the simulated supercell is rather sensitive to the use of single, double and triple moment options of the Milbrandt and Yau scheme. A similar sensitivity to the moment of the MY scheme used was shown for another supercell simulation in Milbrandt and Yau (2006). DXMY10 showed that the DM (and three-moment) MP simulation produced a surface cold pool of strength closer to that observed by the Oklahoma Mesonet (their Figs. 1 and 6) and that the
reflectivity from the DM simulation compared more favorably with observations than that of their SM simulation (DXMY10, their Figs. 6 and 7).

In this study, the output of a 500-m grid spacing, horizontally-homogeneous idealized simulation using the DM version of the MY scheme with α set to zero and using the same sounding as in DXMY10 is used as a “synthetic dataset” to derive the diagnostic relations for \( N_0 \) for each category. This simulation will hereafter be referred to as the MY2 or “reference” simulation. The derived diagnostic relations are then implemented in the SM option of the MY scheme for the various experiments in this study.

Model output of the zeroth and third moments for each precipitating hydrometeor category (rain, snow, graupel, and hail) was taken every 300 seconds throughout the second hour of MY2 and collated into a single large dataset. Data at grid points in the full domain were included in the file, although since vertical grid stretching was employed, the low levels are more heavily sampled than the upper levels. Points were included provided that a minimum threshold of hydrometeor mixing ratio was met. This threshold was purposely kept low at \( 1 \times 10^{-5} \) kg kg\(^{-1} \) for each hydrometeor category, in order to accurately represent the full range of mixing ratios produced by the simulation in the main precipitating region of the storm, while still cutting small, noisy values outside the storm. For each point, the parameters of the inverse exponential distribution were calculated and the mass content \( W \) was derived using

\[
W = 1000 \rho_a q, \tag{6}
\]

where \( W \) is in g m\(^{-3} \), air density \( \rho_a \) is in kg m\(^{-3} \) and mixing ratio \( q \) is in kg kg\(^{-1} \). As in Zhang et al. (2008), we wish to form a power-law relation between \( W \) and \( N_0 \) of the exponential distribution for each species. In our case, these relations are calculated by performing a least squares minimization on both variables to give an effective linear relation between the logarithms of the...
variable pair. Transforming the variables back from logarithmic into linear space provides a power law for \( N_0 \) in terms of \( W \). The coefficient and power of the derived \( N_0-W \) relationships were averaged across the model output times examined in order to give a more general relation for each precipitating hydrometeor category. In addition, the mean \( N_0 \) for each hydrometeor category was computed (Table 1). The plot showing the resulting dependence of \( N_0 \) on \( W \) (along with the time-averaged power-law fit) from the full dataset exhibits a high degree of scatter for rain and hail (Figs.1,4, respectively), and indeed, in the case of rain, the power law fits for individual times varied substantially (Fig. 1, thin dashed lines). Average \( R^2 \) values for rain and hail are accordingly rather low (0.08 and 0.11, respectively). However, the averaged fit for rain (bold dashed line in Fig. 1) represented well the overall trend in the aggregated data. For all other categories, the power law fits for individual times did not vary significantly across the range of times examined (thin dashed lines in Figs. 2-4), which suggests confidence in the robustness of the time-averaged derived relations. Finally, the two-sided p-values, using a hypothesis test where the null hypothesis is that the slope is zero, were very close to zero for all fits, likely due to the large number of points used.

The MY suite of MP schemes contains four frozen hydrometeor categories – ice, snow, graupel and hail – and each of these is handled separately within the ice phase processes. The ice total number concentration, \( N_{iti} \), is already diagnosed based upon temperature in the SM option according to Cooper (1986). For rain and the other three frozen categories, the number concentration is calculated as the zeroth moment of the distribution using \( N_0 \) of the PSD of that species, which is set to a constant value for each species in the original SM MP scheme (see Table 1). Scatter plots showing the dependence of \( N_0 \) on \( W \) for snow, graupel and hail are shown in Figs. 2 through 4. The fixed \( N_0 \) values and the diagnostic power law relations used in the
various SM MY experiments to be discussed in the next section are also shown in the Figs. 1-4. Examining Figs. 1-4 and Table 1, it is clear that for each of the hydrometeor species the coefficient differs significantly from the default fixed value of $N_0$, by up to three orders of magnitude in the cases of snow and graupel.

The time dependence of the coefficient and power in the $N_0$-$W$ relationships were examined (Fig. 5) and no significant time trends were found for any of the four species. It is clear that the rain category demonstrates a great deal of variability in the power of the $N_0$-$W_r$ relation, yet this does not appear to be a function of time.

4. Numerical experiments

In order to test the diagnostic $N_0$ relations, several simulations of the May 3$^{rd}$ 1999 case were performed. The main aim of this study is to implement the diagnostic relations for $N_0$ within a SM MP scheme and determine how well such a SM scheme reproduces the results of DM scheme. We perform several experiments, using the naming convention $MY#X$, where # is the number of moments prognosed, either 1 or 2, and X is a one or two-letter variation identifier, described below and in Table 2. First, the reference DM simulation, $MY2$, is produced and the diagnostic $N_0$-$W$ relations and average $N_0$ values are computed from its output, as described previously. A baseline SM simulation is then produced, using the original MY1 scheme (with the default constant $N_0$ for each category), denoted $MY1A$. The results of the following diagnostic $N_0$ simulations are compared against these to gauge the impact and effectiveness of the diagnostic relations. Two more fixed-$N_0$ simulations were performed: 1) $MY1B$, using the MY1 scheme with $N_0$ lowered from $8 \times 10^6$ m$^{-4}$ to $4 \times 10^5$ m$^{-4}$, and 2) $MY1M$ (“M” for “Mean”), using the average $N_0$ for each category derived from the $MY2$ reference simulation. The reduced value
of $4 \times 10^5$ m$^{-1}$ for $N_{0r}$ in $MYIB$ is 20 times smaller than the default Marshall-Palmer (Marshall and Palmer 1948) DSD value, but is still within the known uncertainty range of $N_{0r}$ (Tong and Xue 2008a), and was also examined in DXMY10 for its impact on the simulation of a supercell storm. The reduced value corresponds to a DSD having more larger drops, which typically leads to less evaporation and a weaker cold pool (DXMY10; Snook and Xue 2008).

Finally, two further simulations were performed using the derived diagnostic-$N_0$ relations, one in which only the rain category used the diagnostic relation, and one in which $N_0$ for all categories, including 4 precipitating hydrometeors total, are diagnosed. These are denoted $MY1DR$ and $MY1DA$ (for “Diagnostic Rain” and “Diagnostic All”), respectively. For each of the SM simulations, the cloud water fixed total number concentration $N_{tc}$ remains at the default value, and again the cloud ice total number concentration $N_{ti}$ is diagnosed based on temperature, as is the default (both $N_{tc}$ and $N_{ti}$ are predicted in $MY2$). Details of the simulations and the nomenclature used can be found in Table 2. The diagnostic functions themselves were applied within the MP scheme (after update by the model dynamics) at the same locations in the code where the original fixed $N_0$ were used for computations. Specifically, in the case of the ice species, this occurs 1) at the beginning of the MP scheme, and 2) just before the call to sedimentation. In the case of rain, additionally the function is applied just before the computation of warm rain processes and again before computation of evaporation.

Each two-hour simulation was performed using the ARPS model with the same single sounding and thermal bubble initialization procedure as in the idealized experiments of DXMY10, and were performed at the same horizontal grid spacing of 500 m. However, in the current study, for efficiency, a reduced domain size of 96x96x20 km was used, and the mean storm motion was subtracted from the original wind profile. Otherwise the setup of the
experiments was identical to that of DXMY10. The use of this idealized model setup allows more control over the experiments, and represents at least part of the natural variability among storms and their environment. It also facilitates direct comparison with the results of DXMY10. In particular, the simulations MY1A and MY2 correspond to MY1 and MY2 from DXMY10.

Fifty-three vertical levels were used with vertical grid stretching employed, giving a vertical grid spacing of 20 m at the surface that decreases to 800 m at the upper boundary. The fourth-order monotonic computational mixing scheme of Xue (2000) was utilized with a coefficient of 0.0015 s\(^{-1}\). The initial ellipsoidal thermal bubble used to trigger the storm had a maximum potential temperature perturbation of 4 K, horizontal radius of 10 km and vertical radius of 1.5 km, and was centered 1.5 km above the surface, 35 km from the west edge and 25 km from the south edge of the domain. The sounding used in the simulation was extracted from a 1-hour forecast of an earlier 3 km real-data simulation of this case, at a location upstream of the low-level inflow of the storms. This was the same sounding used in DXMY10, and full details of the original real-data simulation can be found in Dawson et al. (2007).

Each of the simulations in the current study was run for two hours. Van Weverberg (2013) noted that the short timescale of numerical simulations such as these do not sufficiently cover the entire convective cycle. For this reason, we note that the reported differences between the simulations in the present study may not remain constant over the entire convective cycle.

5. Results and discussion

a. Reflectivity structure

The MY1A simulation produces a storm that by 1 hr displays relatively low reflectivity
values (Fig. 6a\(^1\), max 53 dBZ) in its core, and indeed begins to decay rapidly in the second hour (not shown), due primarily to a relatively strong, surging cold pool (Fig. 9a). It also displays a forward flank region with a relatively small area compared to each of the other experiments (Fig. 6b-f).

In contrast, the forward flank reflectivity region is much larger in MY2 (Fig. 6f) than in MY1A, and is somewhat larger than that typically observed in supercell storms (e.g., Doswell and Burgess 1993). Morrison and Milbrandt (2011) found that the MY schemes produce long and narrow forward flank regions. Further tests (not shown) strongly suggest that this is due to the relatively low fall speed curve of graupel used, but further investigation of this issue is beyond the scope of this paper. This does not affect the key point of this paper since we are primarily interested in how well the results of the SM scheme can match the DM, as a proof-of-concept. However, there are many processes that cannot be well represented within the SM scheme, such as size sorting. In contrast, the DM scheme does parameterize size sorting, although when the shape parameter \(\alpha\) is set to 0 (as in MY2), excessive size sorting tends to occur (MY05a). We suggest that the sharp gradient at the leading edge of the forward flank reflectivity (Fig. 6f) is due to the effect of the excessive size sorting. Simulations of this case performed using the triple-moment MY scheme, which more accurately parameterizes size sorting (MY05a), produced a more gradual and realistic reflectivity gradient in this region (see Fig. 7 in DXMY10), corresponding more closely to radar observations of this case (DXMY10). Additionally, a sensitivity test was performed in which the MY2 experiment was repeated with size sorting turned off (by setting the number-weighted fall speeds equal to the corresponding mass-weighted fall speeds), and this also resulted in a more gradual reflectivity gradient, similar to that of the

\(^1\) In this and similar figures, only a subset of the full model domain is shown.
Both MY1B and MY1M, in which the rain $N_0$ is reduced from MY1A, are seen to produce a storm structure closer to that of MY2 than MY1A does, particularly on the leading edge or forward flank of the storm. The maximum reflectivity in MY1B is 60 dBZ, which is closer to that of MY2 (max 64 dBZ), and significantly increased from that of MY1A. Since the only difference between the MY1B and MY1A is the reduction in the (fixed) value of $N_0r$, this would seem to indicate that the default value of $8 \times 10^6$ m$^{-4}$ for $N_0r$ is too high for the type of severe convective case being simulated here; this is perhaps not surprising as the Marshall-Palmer relation was derived mainly for stratiform rain. For a given water content, increasing $N_0r$ will decrease the median volume diameter, resulting in decreased reflectivity values. Despite the overall structure of the storm being closer to MY2 than MY1A, the areal extent of the forward flank reflectivity region in MY1B is still significantly smaller compared to that in MY2. The areal extent of reflectivity values greater than 30 dBZ at 3600 s is 207 km$^2$ in MY1A, 319 km$^2$ in MY1B, 467 km$^2$ in MY1M, and 1257 km$^2$ in MY2. For a threshold value of 50 dBZ, the corresponding areas covered are 10, 53, 123, and 172 km$^2$, respectively, illustrating the large forward flank region in MY2. The reason for the overall larger regions of higher reflectivity in MY2 is tied to the larger rain sizes predicted in this simulation relative to the others (not shown).

The surface reflectivity structure produced by MY1DR (Fig. 6d) is broadly similar to that of MY1B (Fig. 6b) and MY1M (Fig. 6c), although the lateral extent of the storm is slightly increased. The maximum reflectivity is similar to MY1B, MY1M, and MY2 (Fig. 6b, c, f). The forward flank region in MY1DR shows decreased strength of the east-west reflectivity gradient in the forward flank region (the reflectivity decreases to zero more gradually from west to east) than the fixed $N_0r$ experiments (Fig. 6d), which corresponds more closely to base reflectivity
observations from KTLX (0.5° tilt, not shown). The area with reflectivity greater than 30 dBZ is 474 km$^2$ and that with greater than 50 dBZ is 127 km$^2$.

To investigate possibly closer similarity to the reference simulation $MY2$ in the forward flank region, the diagnostic relations for the $N_0$ of snow, hail and graupel are implemented in $MYIDA$. Examining the reflectivity structure generated by $MYIDA$, (Fig. 6e) it is clear that the inclusion of diagnostic-$N_0$ for graupel, snow and hail has a large effect on the lateral extent of the storm and general storm structure. It was shown by Gilmore et al. (2004) that altering $N_0$ for hail and graupel caused large variations in the accumulated precipitation at the surface, so it is reasonable to expect that altering the values of $N_{0h}$ and $N_{0g}$ should cause changes in several fields. The overall reflectivity structure is seen to resemble that of $MY2$ more closely than any other simulations. Particular increased similarity (relative to the $MY2$ simulation) is noticed in the forward flank region of the storm, with that of $MYIDA$ larger in size than in the other SM simulations. The areal extent of reflectivity $> 30$ (50) dBZ at 3600 s is 686 (166) km$^2$, as compared with 1257 and 172 km$^2$ for $MY2$, respectively. This would suggest that by diagnosing $N_0$ for the frozen categories, we are able to more accurately represent the ice processes that contribute to fall-out from the anvil. We discuss the impact on specific MP processes in section 5e.

While diagnosing $N_{0r}$ produces a simulation closer to $MY2$ than the fixed-$N_{0r}$ SM simulations, the increased similarity is mostly limited to the lowest levels, since the same fixed $N_0$ for the ice categories are used in $MY1DR$ as in $MY1A$, and little change is observed above the freezing level. This can be seen by an examination of the reflectivity structure above the melting level, at 5.5 km height (Fig. 7). $MY1B$ and $MY1DR$ show virtually no differences to $MY1A$ (all have reflectivity magnitudes that are much too high as compared to $MY2$, compare Fig. 7a,b,d.
with Fig. 7f), which is expected as only the rain PSD is altered in these simulations. More specifically, the rain mixing ratios are comparable between MY1A, MY1B, and MY1DR, most of which is converted to hail in the updraft of the storm (not shown). Since, in the SM experiments, only mixing ratio is prognosed, once ice forms aloft, its PSD is dictated solely by its own mixing ratio and \(N_0\), the latter of which is the same fixed value for each ice category in MY1A, MY1B, and MY1DR. In contrast, MY1M and MY1DA both show reflectivity patterns and magnitudes much closer to that of MY2, (max reflectivities at 3600 s of 53, 52, and 47 dBZ, respectively, Fig. 7c,e,f) demonstrating the value of either using the mean or diagnosed \(N_0\) for the ice categories.

Although the reflectivity structure at only a single time has been shown for the sake of brevity, the structure at other times is qualitatively consistent with the above analysis (not shown). Nevertheless it is instructive to examine the temporal evolution of the behavior in reflectivity. This is accomplished by computing the RMS difference at the surface for each of the SM simulations against that of MY2, for the duration of the 2 hr simulations. The results are shown in Fig. 8. Consistent with the analysis of the plots at 3600 s above, MY1DA is closest to MY2 for the entire duration of the simulation period, showing the largest area of moderate reflectivity relative to MY2 (Fig. 8a), and the lowest RMS difference of all the SM experiments (Fig. 8b). In contrast, MY1A clearly performs poorly across the entire simulation duration.

b. Cold pool structure

The cold pool is discussed in terms of the equivalent potential temperature perturbation \((\theta'_e)\) fields at the surface, as in DXMY10, since the \(\theta'_e\) field also takes into account moisture effects. Here, \(\theta_e\) is calculated according to Bolton (1980).

The cold pool produced in MY1A is seen to be rather strong (Fig. 9a), with a minimum \(\theta'_e\) of -29 K at 3600 s. The areal extent of the cold pool as defined by a threshold of \(\theta'_e < -1\) K also
continues to increase with time during the simulation period (Fig. 10a). In fact, it is the strength of the cold pool which cuts off the updraft after one hour and causes the simulated storm to decay (not shown). In addition to having the largest $\theta_e'$ deficit, the areal extent of the cold pool at 3600 s is also the largest of any of the simulations, at 557 km$^2$. The time evolution of the cold pool in each experiment is quantified in Fig. 10, which shows total cold pool area as defined above (Fig. 10a), minimum $\theta_e'$ (Fig. 10b), and RMSD of surface $\theta_e$ relative to the reference experiment MY2. MYIA consistently shows the largest cold pool area, smallest minimum $\theta_e'$, and highest RMSD of $\theta_e$ of any of the experiments.

The cold pool in MY2 is very weak in comparison, with a minimum $\theta_e'$ of -10 K, which is comparable to the minimum $\theta_e'$ observed by the mobile mesonet (Markowski 2002). The areal coverage of $\theta_e' < -1$ K at 3600 s is substantially less than in MYIA, at 205 km$^2$.

The cold pool produced by MYIB is weaker than that of MYIA, with a maximum $\theta_e$ deficit of -24 K, and an areal coverage of $\theta_e' < -1$ K of 358 km$^2$ at 3600 s. Several researchers (e.g., Milbrandt and Yau 2006; Snook and Xue 2008; DXMY10) found that simulations performed using reduced values for $N_0r$ and $N_0h$ tend to produce a relatively weak cold pool when compared to simulations performed using increased $N_0$ values. This behavior is due to distributions that favor fewer large particles possessing a reduced total hydrometeor surface area when compared to the same mass of water distributed as a large number of smaller particles. This reduced surface area limits the potential for evaporative and melting cooling, which are important mechanisms for cold pool formation.

The cold pool structure of MYIDR at 3600 s is rather similar to that of MYIB in terms of both maximum strength and areal coverage (compare Fig. 9b to d), and its time evolution is also remarkably similar (Fig. 10 solid gray and black dashed lines, respectively). This indicates that
simply reducing $N_0r$ by a factor of 20 produces much the same benefit in this case as diagnosing $N_0r$ in terms of the cold pool structure and intensity. While a considerable decrease in cold pool strength is seen from MY1A to MY1DR, the further decrease in cold pool strength from MY1DR to MY1DA would suggest that the frozen categories have a comparable impact (as demonstrated for graupel in Van Weverberg et al. 2012). It is suggested that as the diagnostic relation changes the shape of the frozen categories PSD, this modulation is reflected in changes in processes such as melting, and collection of rain by hail. Using melting as an example, note, however, that in the case of the SM schemes the PSD of rain depends only on its unique $N_0$-$W$ relation (whether fixed or diagnosed) and not on the PSD of the melting category, whereas the same is not generally true for a DM scheme.

Finally, simulations MY1M and MY1DA, which involve using the fixed $N_0$ for each species using the mean value computed from MY2, and using the diagnostic relations derived from MY2, respectively, also show remarkably similar cold pool structure and intensity at 3600 s (Fig. 9c,e). Both also compare very favorably to the MY2 cold pool at this time (Fig. 9f). The time evolution of total cold pool area and minimum $\theta_e$ is also closest to MY2 of any of the other SM simulations (Fig. 10a,b), while both have nearly identical RMS differences in $\theta_e$ against MY2 (Fig. 10c).

From these results, either choosing more accurate fixed values of $N_0$ or the diagnostic approach clearly shows promise in producing cold pools closer to the DM results. Although reducing the strength of the cold pool is clearly not desirable in all cases, the goal of this study is to recreate the key features of the DM scheme, which in this case presented with a cold pool of significantly reduced strength from the default SM (MY1A) simulation.
c. Total number concentration

The striking differences in storm structure and cold pool between the experiments in this study exemplify the large impact that PSD parameters can have upon the simulation results. As demonstrated previously altering $N_0$ affects the simulation indirectly through feedback from processes such as evaporative effects, but also directly through the impact on $N_r$. An important test of the viability of the diagnostic-$N_0$ approach is to investigate how well the $N_r$ fields are reproduced relative to the MY2 experiment, which explicitly predicts $N_r$ ($N_r$ in the single moment schemes is diagnosed from $q$ and $N_0$ for a given category). Following the approach above, we present plots of the rain total number concentration $N_{rr}$ at the surface at 3600 s for each of the experiments in Fig. 11. Immediately it can be seen that there are large variations in the both the magnitude and range of $N_{rr}$ values across each of the single moment simulations. In general, the diagnostic-$N_{0r}$ simulations, MY1DR and MY1DA (Fig. 11d,e) compare most favorably in a qualitative sense with MY2 (Fig. 11f), particularly when considering the range of values from the core to the edge of the forward flank. In contrast, MY1A, MY1B, and MY1M (the fixed-$N_0$ simulations) all have a much different range of $N_{rr}$ across the storm, although MY1B shows the closest maximum value of $N_{rr}$ as compared with MY2 (462 m$^{-3}$ and 342 m$^{-3}$, respectively). This behavior is reflected in the histograms of $N_r$ shown in Fig. 12, which confirm that the diagnostic-$N_0$ simulations better capture the range and shape of the distribution of $N_r$ in the simulations for each of the hydrometeor categories, while the fixed-$N_0$ simulations have histograms that, depending on the choice of the fixed value of $N_0$ in each case, exhibit only partial overlap with the range of values from MY2 (e.g. as in the case of $N_{rr}$ for MY1A as compared with MY2, Fig. 12a). In general, none of the SM schemes fully capture the broad range of $N_r$ values exhibited by
the MY2 scheme for each category, but the diagnostic relations clearly outperform the fixed-$N_0$
simulations in this regard.

We note here that even though similar results, in terms of the cold pool strength and
precipitation structure, seem obtainable by choosing a reasonable fixed value of the rain $N_0$ (such
as in MY1B and MY1M), in practice, it is difficult to predetermine what value should be used and
the constant fixed values are not necessarily realistic, as is shown above when considering the
histograms of $N_r$. For this reason, we believe the diagnostic relations hold more promise; to say
the least they provide spatial variability to the PSD parameters that should more realistic than
assigned constant values.

In terms of each of the variables examined in this study, consistent increase in similarity
to MY2 is seen in MY1DR over MY1M, MY1B, and MY1A, in that order. Further similarity to
MY2 in examined variables is seen in MY1DA, consistent with the goal of this study. This is
encouraging, and it is suggested that the method of diagnosing $N_0$ based on independently
predicted variables merits further investigation. We suggest that the diagnostic relationships be
derived for additional cases besides supercells to investigate the representativeness of the
relations derived in this study. An investigation into the dependence of the diagnostic relations
on variables other than water content, such as temperature and updraft velocity, would also add
value to this method. Although a diagnostic relation for $N_0$ brought the simulation results closer
to the DM results, we recognize that there is a limit to this approach; there are intrinsic limits to
the SM scheme. One example of these limits can be seen by examining carefully the pattern of
$N_r$ in MY2 (Fig. 11f), which exhibits a dipole structure approximately straddling the centerline of
the forward flank reflectivity region, with higher values to the north of this line, and
progressively smaller values to the south. This gradient in $N_r$ is associated with larger mean
diameters of rain near the south edge of the forward flank, and progressively smaller mean
diameters toward the north (not shown), which is consistent with observed and simulated $Z_{DR}$
arcs (e.g., Kumjian and Ryzhkov 2008, 2009, 2012; Jung et al. 2010; Snyder et al. 2010). This
pattern is a reflection of raindrop size sorting, which again comes about in MY2 due to the
differential sedimentation of the $q$ and $N_i$ moments (e.g., MY05a). In contrast, each of the SM
simulations, including the diagnostic-$N_0$ simulations, shows a monopole pattern in $N_{tr}$, with the
maximum located near the maximum in reflectivity near the core of the storm; the diagnostic
relation for $N_0$ cannot fully represent all complex physical processes included in the DM scheme,
including size sorting.

d. Squall line case

Since the diagnostic relations were derived from a DM simulation of a supercell storm,
the relative increase in similarity between the results of MY1DA and MY1DR to MY2 as
compared to MY1A (shown in sections 5a-5c) is perhaps not that surprising. A question one
would ask is if these relationships are applicable to other types of convective systems, such as
the squall line. To answer this question, we apply the diagnostic relations obtained above to a
simulated squall line.

The squall line is again simulated using the ARPS model, in two dimensions. The domain
is 700 km in the x-direction and 20 km in the vertical. The grid spacing is 1 km in the horizontal.
In the vertical there are 64 levels, with the vertical grid spacing being 100 m in the lowest 3 km,
and gradually increasing to 850 m at the model top. The simulations use the Weisman and
Klemp (1982) analytic thermodynamic sounding. The wind profile used is -17.5 m s$^{-1}$ at the
surface, decreasing linearly to 0 m s$^{-1}$ at a height of 5 km, giving 17.5 m s$^{-1}$ of shear within the
lowest 5 km. The wind speed remains zero above 5 km.
For the squall line, three separate simulations were run. The first simulation uses the original SM MY MP scheme and is denoted $MY1A-Q$ (corresponding to $MY1A$). The second simulation uses the DM MY MP scheme (denoted $MY2-Q$, corresponding to $MY2$). The final simulation used the diagnostic-$N_0$ relations defined in Section 3 for rain, snow, graupel, and hail. This simulation is denoted $MY1D-Q$ and corresponds to $MY1D$. Each of these three simulations was run for twelve hours.

The reflectivity fields shown in Fig. 13 represent the averages (relative to the leading edge of the surface gust front) over hours 3-6 of model time (note that this represents a mature squall line; in all cases the squall line becomes mature and quasi-steady by 3 hours into the simulation). The $MY1A-Q$ simulation shows a strong cold pool and a rearward-tilted updraft, with the maximum updraft in the lower levels (Fig. 13a). $MY2-Q$ shows a weaker, more elevated updraft, with a tilt close to neutral and a weaker cold pool (Fig. 13c). The mean reflectivity in $MY1D-Q$ shows a similar structure to that of $MY2-Q$, with a neutrally-tilted updraft, and the updraft maximum in the mid-levels (as opposed to the lower levels in $MY1A-Q$; Fig. 13b). The height of the maximum reflectivity is within the lowest 3km in both $MY1D-Q$ and $MY2-Q$, whereas the column of maximum reflectivity in $MY1A-Q$ reaches a height of 7 km. The strong increase in reflectivity immediately below the melting layer in $MY1D-Q$ suggests a more vigorous cold rain process, which is not seen in $MY2-Q$, suggesting that the diagnostic approach may not be optimally tuned for the squall line case.

The cold pool in $MY1D-Q$ is weaker than either $MY1A-Q$ or $MY2-Q$. This can be seen in more detail in Fig. 14, which shows the time evolution of the surface cold pool in each of the simulations. It is clear that while the cold pool is weakest in $MY1D-Q$, the cold pool evolution
is closer to that of MY2-Q than MY1A-Q, which shows continued eastward growth after two hours of simulation time, although MY1A-Q and MY2-Q do not.

While the results from MY1A-Q more closely resemble those of MY2-Q than did those of MY1A-Q, this does not necessarily mean that the MY1A-Q results are more realistic. In fact, comparisons with the conceptual model for squall line MCSs presented in Houze (2004) suggest that the strong increase in reflectivity immediately below the melting level in Fig. 13 is not physically realistic. We do have the need to further test the diagnostic relations for \( N_0 \) with cases encompassing a range of precipitation types though.

e. Sensitivity of MP processes to the diagnostic relations

To better understand the seemingly enhanced similarity of the simulations performed using the diagnostic relations to the DM simulations over the original SM simulations, we examine here how the diagnostic relations affect certain MP process rates for a range of mixing ratio values from the supercell simulations. The \( N_0 \) values are set as follows: for the original SM scheme, constant values are used for all species (solid black lines in Figs. 1-4). For the diagnostic scheme, \( N_0 \) is diagnosed for each species using the relations derived in Section 3. For the DM simulation, the \( N_0-W \) pairs from MY2 are sampled throughout the model domain over the entire range of times used to derive the diagnostic relations (see section 3).

Four MP processes are examined: rain evaporation, melting of snow, graupel, and hail. To examine these processes, the three sets of \( q-N_0 \) values defined above are used in the calculations of the equations of corresponding processes, taken from the MY schemes within the ARPS model. Each process is computed at a constant temperature of 5°C, an air density of 1 kg m\(^{-3}\), and a water vapor mixing ratio of 5 g kg\(^{-1}\). The results (Fig. 15) show that for each of the processes examined, the diagnostic-\( N_0 \) better fits the envelope of points from the DM scheme.
than the original fixed-$N_0$ SM scheme does. For each of the processes, the fixed $N_0$ results in a line that does not overlap the set of points from the DM scheme (Fig 15a-f). That the diagnostic scheme line lies close to or within the spread of $q-N_0$ from the DM scheme serves to explain the similarity between the cold pool structure from $MYIDA$ and $MY2$ (and $MYIDA-Q$ and $MY2-Q$).

Since the MP processes seem to be better represented (“better” in terms of being “closer to the $MY2$ reference”) in $MYIDA$, we suggest that the use of the diagnostic-$N_0$ method holds promise for simulations of other types of storms also.

6. Summary and conclusions

The overall goal of this study was to establish and utilize a relationship between the PSD parameters and the hydrometeor mass variables typically predicted in SM MP schemes in the hope of producing results closer to those of DM schemes. The PSD parameter chosen was the intercept parameter $N_0$. It has already been shown from disdrometer measurements that there is a measurable positive correlation between the two variables (Zhang et al. 2008) and in this study we derived such relationships based on the output of an idealized two-moment simulation. The original SM Milbrandt and Yau MP scheme uses a fixed value for $N_0$ for each hydrometeor species. Two control simulations were run using the original single ($MY1A$) and DM ($MY2$) MP schemes and these were used as the basis against which all subsequent simulations in this study are compared.

Simply reducing the fixed value of $N_{0r}$ by a factor of 20 ($MY1B$) showed improvements over $MY1A$ in terms of producing results more closely aligned with those of the DM simulation (more realistic reflectivity structure, reduced cold pool strength, reduced number concentration.)

Diagnosing $N_{0r}$ ($MY1DR$) produced simulations more consistent with $MY2$ than did the original fixed-$N_{0r}$ SM simulation $MY1A$. However, these are limited to the lowest levels. The
addition of a diagnostic relation for \( N_0 \) for the frozen hydrometeor categories (MYIDA) brings the simulation results further in line with MY2 than when \( N_0 \) only is diagnosed. Results with further increased consistency with MY2 are seen at low levels as well as above the melting layer, due to increased consistency with MY2 in the structure of the frozen categories that can cause changes in the rain category through fallout and melting, among other processes.

The use of diagnostic relations for several frozen species was found to significantly increase the lateral extent of the storm in MYIDA over the other SM simulations. Extending the diagnostic-\( N_0 \) relation to the frozen hydrometeors also has a large positive impact on the cold pool structure. It is known that altering \( N_0 \) of any of the hydrometeor distributions can have a large effect on the cold pool, as altering the shape of the distribution directly affects the rate of evaporative or melting cooling (e.g., Gilmore et al. 2004; van den Heever and Cotton 2004; Milbrandt and Yau 2006; Snook and Xue 2008; Dawson et al. 2010).

While MYIDR produced a cold pool smaller in size and strength than that of MYIA, diagnosing the frozen category \( N_0 \) further reduced both the intensity and size of the cold pool, bringing the temperature deficit in line with that of MY2. The cold pool in MY2 was very weak, which agrees well with surface mesonet observations from the event (Markowski 2002), hence the decreased cold pool strength through diagnosing \( N_0 \) of the frozen species is encouraging.

Although the improved consistency of MYIDA with MY2 (as compared to MYIA) is encouraging, the diagnostic relations require testing to ensure that the derived relations are not too case-specific. Similar results were obtained for the simulations of a 2-D squall line. Using the diagnosed \( N_0 \) relations obtained from the reference supercell simulation, the reflectivity structure and cold pool evolution of the SM simulation were brought closer to the results of the DM simulation for the squall line case also. An examination of four specific MP processes
(evaporation of rain, and melting of snow, graupel, and hail) using the diagnostic relations showed that their use brought the rates of all four processes closer to the rates evaluated using the DM scheme.

Although further testing is needed over a wider range of cases (e.g., severe convective storms, stratiform precipitation, and winter storms), the method examined in this paper shows considerable promise in bringing the results of a six-prognostic-variable SM MP scheme closer to a DM MP scheme, with a considerably lower computational cost compared to the DM scheme.

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Fig. 2. As in Fig. 1, but for snow.

Fig. 3. As in Fig. 1, but for graupel.

Fig. 4. As in Fig. 1 but for hail.

Fig. 5. Variation with time of the coefficient \((A\), upper panel\), and power \((b\), middle panel\) in the \(N_0=Ax^b\) relation for each of the four hydrometeor species considered. The lower panel shows the number of points used to determine the relations for each species.

Fig. 6. Reflectivity (color fill) and horizontal wind vectors at the surface (plotted every 2.5 km) for a subset of the domain at 3600 s into the six simulations: a) \(MY1A\), b) \(MY1B\), c) \(MY1M\), d) \(MY1DR\), e) \(MY1DA\), and f) \(MY2\).

Fig. 7. As in Fig. 5 but for an altitude of ~5680 m.

Fig. 8. Area of surface reflectivity > 30 dBZ versus time for each of the experiments (a) and RMS difference in surface reflectivity from experiment \(MY2\) versus time for each of the single-moment experiments (b).
Fig. 9. As in Fig. 5 but for surface equivalent potential temperature perturbation (color filled) and reflectivity (contours, 10 dBZ increment).

Fig. 10. Evolution of (a) total area of the cold pool as defined by all grid squares at the surface with $\theta_e' < -1$ K for each simulation, (b) the minimum $\theta_e'$ in the cold pool for each simulation, and (c) the RMS difference in $\theta_e$ for each of the five single-moment simulations when compared to MY2.

Fig. 11. As in Fig. 5 but for rain total number concentration $N_r$ (m$^{-3}$, color filled).

Fig. 12. Normalized histograms of (a) rain, (b) snow, (c) graupel, and (d) hail total number concentration $N_t$ for (red) MY2, (blue) MY1A, (cyan) MY1B, (green) MY1M, (orange) MY1DR, and (purple) MY1DA. Note the logarithmic scale for both axes. Histograms represent the accumulation of all grid points with $q > 1.0 \times 10^{-5}$ kg kg$^{-1}$ from 3600 to 7200 s at 300 s intervals for each simulation.

Fig. 13. Reflectivity (color filled), wind vectors (every 10 km in horizontal, every 4$^\text{th}$ level in the vertical), vertical velocity (gray contours, only 1 m s$^{-1}$ and 5 m s$^{-1}$ shown), and potential temperature perturbations (dashed blue contours, 1 K increment) averaged over hours 3-6 of the three squall line simulations: a) MY1A-Q, b) MY1DA-Q, and c) MY2-Q.

Fig. 14. Perturbation potential temperature $\theta'$ at the surface versus time (color filled), to show the evolution of the cold pool in the three squall line simulations: a) MY1A-Q, b) MY1DA-Q, and c) MY2-Q.

Fig. 15. The effect of the diagnostic intercept parameter on select MP processes: a) rain evaporation, b) snow melting, c) graupel melting, and d) hail melting. For each process, the results using three MP schemes are shown: MY1A (black line), MY1DA (red line) and MY2 (blue crosses).
Table 1. The fixed $N_{0x}$ values used in the original MY single-moment microphysics scheme, the derived diagnostic relation for $N_{0x}$, and the mean $N_{0x}$ values from simulation MY2 for rain, snow, graupel and hail.

<table>
<thead>
<tr>
<th>Species</th>
<th>Default fixed $N_{0x}$ values</th>
<th>Diagnostic relation derived from MY2 simulation</th>
<th>Mean $N_{0x}$ from MY2 simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rain</td>
<td>$N_{0r} = 8 \times 10^6 \text{ m}^{-4}$</td>
<td>$N_{0r} = 1.16 \times 10^5 W_r^{0.477} \text{ m}^{-4}$</td>
<td>$N_{0rm} = 1.18 \times 10^5 \text{ m}^{-4}$</td>
</tr>
<tr>
<td>Snow</td>
<td>$N_{0s} = 3 \times 10^6 \text{ m}^{-4}$</td>
<td>$N_{0s} = 4.58 \times 10^5 W_s^{0.788} \text{ m}^{-4}$</td>
<td>$N_{0sm} = 3.95 \times 10^8 \text{ m}^{-4}$</td>
</tr>
<tr>
<td>Graupel</td>
<td>$N_{0g} = 4 \times 10^5 \text{ m}^{-4}$</td>
<td>$N_{0g} = 9.74 \times 10^8 W_g^{0.816} \text{ m}^{-4}$</td>
<td>$N_{0gm} = 5.26 \times 10^7 \text{ m}^{-4}$</td>
</tr>
<tr>
<td>Hail</td>
<td>$N_{0h} = 4 \times 10^4 \text{ m}^{-4}$</td>
<td>$N_{0h} = 5.25 \times 10^5 W_h^{0.411} \text{ m}^{-4}$</td>
<td>$N_{0hm} = 3.50 \times 10^5 \text{ m}^{-4}$</td>
</tr>
</tbody>
</table>
Table 2. Description of the microphysical setup used in the six simulations that were performed at 500-m horizontal resolution.

<table>
<thead>
<tr>
<th>Experiment Name</th>
<th>Details of microphysics scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>MY2</td>
<td>Original double-moment Milbrandt and Yau scheme.</td>
</tr>
<tr>
<td>MY1A</td>
<td>Original single-moment Milbrandt and Yau scheme.</td>
</tr>
<tr>
<td>MY1B</td>
<td>Single-moment with reduced fixed value of $N_0 = 4 \times 10^5$ m$^{-4}$.</td>
</tr>
<tr>
<td>MY1M</td>
<td>Single-moment with intercept parameter set to mean values from MY2 for all precipitating hydrometeor categories.</td>
</tr>
<tr>
<td>MY1DR</td>
<td>Single-moment with intercept parameter diagnosed for rain only.</td>
</tr>
<tr>
<td>MY1DA</td>
<td>Single-moment with intercept parameter diagnosed for all precipitating hydrometeor categories.</td>
</tr>
</tbody>
</table>
Fig. 1. Scatterplot and fits of rain intercept parameter ($N_{or}$) vs. water content ($W_r$) from MY2. For clarity only every 100th point used in the fits are plotted. The $N_{or}$-$W_r$ pairs are directly computed from the predicted zeroth and third moments of the exponential DSD. The bold dashed line shows the average derived fitted relation (in linear space), thin dashed lines show the derived fits for individual times (every 300 s in the second hr of the simulation), the solid line shows the original fixed value of $N_{or}$ used in the MY1A experiment, the dash-dotted line shows the reduced $N_{or}$ used in experiment MY1B, and the dotted line shows the mean $N_{or}$ (from MY2) used in experiment MY1M.
Fig. 2. As in Fig. 1, but for snow.
Fig. 3. As in Fig. 1, but for graupel.

\[ N_{0g} = 9.74 \times 10^8 W_g^{0.816} \]

\[ R^2 = 0.51 \]
Fig. 4. As in Fig. 1 but for hail.

$$R^2 = 0.11$$

$$N_{0h} = 5.25 \times 10^5 W_h^{0.411}$$
Fig. 5. Variation with time of the coefficient ($A$, upper panel), and power ($b$, middle panel) in the $N_0=Ax^b$ relation for each of the four hydrometeor species considered. The lower panel shows the number of points used to determine the relations for each species.
Fig. 6. Reflectivity (color fill) and horizontal wind vectors at the surface (plotted every 2.5 km) for a subset of the domain at 3600 s into the six simulations: a) MY1A, b) MY1B, c) MY1M, d) MY1DR, e) MYIDA, and f) MY2.
Fig. 7. As in Fig. 6 but for an altitude of ~5680 m.
Fig. 8. Area of surface reflectivity > 30 dBZ versus time for each of the experiments (a) and RMS difference in surface reflectivity from experiment MY2 versus time for each of the single-moment experiments (b).
Fig. 9. As in Fig. 6 but for surface equivalent potential temperature perturbation (color filled) and reflectivity (contours, 10 dBZ increment).
Fig. 10. Evolution of (a) total area of the cold pool as defined by all grid squares at the surface with $\theta_e' < -1$ K for each simulation, (b) the minimum $\theta_e'$ in the cold pool for each simulation, and (c) the RMS difference in $\theta_e$ for each of the five single-moment simulations when compared to MY2.
Fig. 11. As in Fig. 6 but for rain total number concentration $N_{tr}$ (m$^{-3}$, color filled).
Fig. 12. Normalized histograms of (a) rain, (b) snow, (c) graupel, and (d) hail total number concentration $N_t$ for (red) MY2, (blue) MY1A, (cyan) MY1B, (green) MY1M, (orange) MY1DR, and (purple) MY1DA. Note the logarithmic scale for both axes. Histograms represent the accumulation of all grid points with $q > 1.0 \times 10^{-5}$ kg kg$^{-1}$ from 3600 to 7200 s at 300 s intervals for each simulation.
Fig. 13. Reflectivity (color filled), wind vectors (every 10 km in horizontal, every 4th level in the vertical), vertical velocity (gray contours, only 1 m s$^{-1}$ and 5 m s$^{-1}$ shown), and potential temperature perturbations (dashed blue contours, 1 K increment) averaged over hours 3-6 of the three squall line simulations: a) $MY1A$-$Q$, b) $MY1DA$-$Q$, and c) $MY2$-$Q$. 
Fig. 14. Perturbation potential temperature $\theta'$ at the surface versus time (color filled), to show the evolution of the cold pool in the three squall line simulations: a) $MY1A-Q$, b) $MY1DA-Q$, and c) $MY2A-Q$. 
Fig. 15. The effect of the diagnostic intercept parameter on select MP processes: a) rain evaporation, b) snow melting, c) graupel melting, and d) hail melting. For each process, the results using three MP schemes are shown: MY1A (black line), MY1DA (red line) and MY2 (blue crosses).