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7 **Diagnosing the Intercept Parameters of the Exponential Drop Size Distributions in a**
8 **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 of the exponential particle size distribution and the water content for the rain, hail, graupel and snow hydrometeor categories. The derived relations are implemented 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 single- and double-moment versions of the microphysics schemes. Diagnosing the intercept parameter 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. Improvements were 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 alignment with the double-moment simulation results. The decreased cold pool intensity is very similar to that produced by the double-moment simulation, and the areal extent of the storm is more accurately reproduced. This study suggests that significant improvements over traditional fixed-intercept parameters in typical single-moment microphysics schemes can be achieved through the use of diagnostic relations for the parameters of the particle size distribution, without a significant increase in computational cost.

1. Introduction

As numerical weather prediction (NWP) models gain convection-resolving resolutions of 1 km and higher, the parameterization of microphysical processes becomes critical, especially for precipitation forecasts. Generally, bulk microphysics 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

$$N(D) = N_0 \exp(-AD), \quad (1)$$

where N_0 is the intercept parameter and A is the slope parameter of the PSD. Usually the intercept parameter is assigned a fixed value in single-moment microphysics schemes. The most well-known of these exponential distributions is the Marshall-Palmer (Marshall and Palmer 1948) distribution, which specifies N_0 to be 8×10^6 drops m^{-4} for rain. However, using this fixed value for the rain intercept parameter has been shown to be restrictive, as the intercept parameter can vary significantly within single precipitation events both spatially and temporally (Tokay and Short 1996; Zhang et al. 2008). Snook and Xue (2008) investigated the effect of varying N_0 for the rain and hail particle size distributions (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, the resulting cold pools were weaker and the simulations tended to develop into single or multiple supercells, while when N_0 was raised, 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 slope parameter 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, Van Weverberg et al. (2010; 2011a) also investigated the impact of PSDs in single-moment microphysics scheme on precipitation and storm dynamics, and the sensitivity of simulated precipitation systems to microphysics complexity (Van Weverberg et al. 2011b).

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

$$N(D) = N_0 D^\alpha \exp(-AD), \quad (2)$$

where α is the shape parameter, a dimensionless measure of the spectral width of the distribution. If α 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.

Each of the parameters of the gamma distribution varies widely in value in nature, thus parameterizing any of them as constant will introduce a source of error into the microphysics. Ulbrich (1983) calculated a typical range of values for α 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 α varied from -3.42 to 5.04 (the range was far narrower for studies

based on convective rain, with α 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 and Milbrandt and Yau 2005a,b).

The role of the shape parameter α was investigated in detail by Milbrandt and Yau (2005a), who showed that the rate of gravitational particle size sorting was dependent on α , with the size sorting rate decreasing as α increases and approaching 1 as α becomes large. Size sorting is an intrinsic process within supercell evolution, as witnessed by the occurrence of the differential reflectivity (Z_{DR}) arc within supercells. Kumjian and Ryzhkov (2008, 2009) found that the Z_{DR} arc is associated with large, oblate raindrops and relatively few small drops, suggesting that size-sorting is responsible for the modification of the DSD. Hence it is important to parameterize the PSD in a realistic manner, allowing all parameters to vary as appropriate.

A way to improve a microphysics scheme is to increase the number of predicted moments of the PSD (Straka and Mansell 2005; Milbrandt and Yau 2005a). How the moments of the PSD are calculated depends on the way the PSD is parameterized. For the gamma distribution the n^{th} moment is calculated as

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

Most bulk microphysics schemes, especially those used in operational NWP models, only predict one moment of the distribution, typically the third moment M_3 , which is proportional to the hydrometeor mixing ratio, q_x (here x denotes one of the species). In this case, it is usually the slope parameter A that is effectively prognostic while N_0 and α are held constant (with α fixed at 0 for the inverse exponential distribution), although in a Thompson et al. (2004) simulation the

intercept parameter for snow is diagnosed based on temperature. More recently, microphysical schemes that predict two or more moments have become increasingly popular, particularly for convective scale modeling. Most of the double-moment schemes available predict both the mixing ratio and number concentration, leaving α held constant while N_0 and Λ are directly linked to the predicted variables (e.g., Milbrandt and Yau 2005a; Morrison et al. 2005).

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 et al. (2008), gathered in central Oklahoma during the summers of 2005 through 2007, to derive a relationship between the intercept parameter of the inverse exponential PSD and the rain water content (which 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 $N_0(M_2, M_4) = 7106 W^{0.648}$, where N_0 is measured in $\# \text{ m}^{-3} \text{ mm}^{-1}$ and W is in g m^{-3} . Here N_0 is given as a function of M_2 and M_4 because its relation is derived from these two moments.

In the single-moment version of the Milbrandt and Yau microphysics scheme (Milbrandt and Yau 2005b, hereafter MY), 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 α .

In this paper, we assume α to be zero, leading to the exponential distribution commonly used in single moment schemes.

Given the moment relation in (3) and setting α to zero, we see that the exponential PSD parameters, N_0 and Λ , 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

$$N_0 = \frac{M_j \Lambda^{j+1}}{\Gamma(j+1)}, \quad (4)$$

$$\Lambda = \left[\frac{M_j \Gamma(k+1)}{M_k \Gamma(j+1)} \right]^{\frac{1}{k-j}}. \quad (5)$$

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

The goal of this study is to formulate and test diagnostic relationships between the intercept parameter and water/ice content for each precipitating hydrometeor species, and implement this within the single-moment MY microphysics scheme (Milbrandt and Yau 2005b) available within the ARPS nonhydrostatic model (Xue et al. 2000; Xue et al. 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 improve the results of the single-moment

microphysics scheme for them to be closer to the results of the corresponding double-moment microphysics 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 double-moment MY microphysics 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 Milbrandt and Yau double-moment simulations to derive the relations. We use a realistic simulation of a real tornadic supercell storm for the test. The case is described next.

The remainder of the paper is organized as follows: the case being simulated is described in section 2. The formulation of the diagnostic intercept parameter 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. The storm that produced the F5 tornado is the focus of this study.

Observations from the Oklahoma Mesonet (Brock et al. 1995) indicated that the cold pools associated with the supercell which produced the F5 tornado were mainly small and relatively weak. The synoptic setup for the event has been discussed in detail 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. Dawson et al. (2010) simulated a supercell storm within an environment believed to be representative of the environment that storm A developed, and the study found significant sensitivity of the simulated supercell storm to the number of moments predicted with versions of the MY scheme. The predicted cold pool was generally too strong with the single moment scheme while the simulation of the three-moment scheme was found to be the best.

3 Diagnostic relations for intercept parameters

The ARPS implementation of the double-moment MY microphysics scheme has two options, schemes 2 and 2a (hereafter referred to as MY2 and MY2a). Scheme 2 fixes the shape parameter of the gamma distribution, α , to a constant value; when α is set to zero this reduces to the inverse exponential distribution. Scheme 2a diagnoses α for each sedimenting hydrometeor species based upon the mean mass diameter D_{mx} , in the form $\alpha_x = c_{1x} \tanh [c_{2x} (D_{mx} - c_{3x})] + c_{4x}$,

where D_{mx} is in units of mm and c_{1x} through c_{4x} are empirically determined coefficients, detailed in their Table 1 (Milbrandt and Yau 2005a), allowing variability in the PSD shape.

As pointed out earlier, 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 double-moment simulation for the May 3, 1999 case to derive diagnostic relations for use in a single-moment scheme. This allows us to see how close the results of single-moment scheme with diagnostic relations can be to those of double-moment scheme.

Using a single sounding to define the storm environment, Dawson et al. (2010) have shown for the May 3, 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). Dawson (2009) further performed more realistic simulations of this case using 3D inhomogeneous initial conditions that included the assimilation of radar data. The simulation used three levels of nested grids, at 3 km, 1 km and 250 m horizontal grid spacings, respectively. The North America Regional Reanalysis (NARR) provided the initial analysis background and the boundary conditions for the outermost 3 km grid. The assimilation of Oklahoma City WSR-88D (KTLX) radar data was performed on the 1 km grid, using ARPS Data Analysis System (ADAS) (Brewster 1996) that includes a complex cloud analysis component. The cloud analysis makes use of satellite and radar observations to define cloud and hydrometeor fields and adjust in-cloud temperature and moisture fields (Hu et al. 2006). Conventional observations were analyzed using a successive correction scheme that converges to an optimal interpolation solution (Brewster 1996; Lazarus et al. 2002). These simulations were performed using a full set

of physics in the ARPS (Xue et al. 2001). Details of these simulations can be found in Dawson (2009).

In this study, the output of the 250 m simulation using the MY2 scheme with α set to zero from that study is used as a “synthetic dataset” to derive the diagnostic relations for the intercept parameters. This simulation will hereafter be referred to as the “reference” simulation. The simulation using MY2 instead of MY2a is chosen as the reference to avoid the complication of non-zero α that changes the physical interpretation or even the unit of the intercept parameter. The derived diagnostic relations are then implemented in the single-moment option of the MY scheme for the various experiments in this study.

Model output was taken every 300 seconds throughout the second hour of the reference simulation and collated. For each of the thirteen times, a file containing the zeroth and third moment was produced for each precipitating hydrometeor category, which in the Milbrandt and Yau suite of microphysics schemes includes rain, snow, graupel and hail. 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 $1 \times 10^{-5} \text{ kg kg}^{-1}$ for rain and $5 \times 10^{-5} \text{ kg kg}^{-1}$ for snow, graupel and hail, in order to accurately represent the full range of mixing ratios produced by the simulation. For each point, the parameters of the inverse exponential distribution were calculated and the mass content W was derived using

$$W_x = 1000 \rho_a q_x, \quad (6)$$

where W_x is in g m^{-3} , air density ρ_a is in kg m^{-3} and mixing ratio q_x is in kg kg^{-1} . As in Zhang et al. (2008), we wish to form a power-law relation between the water content and the intercept

parameter 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_{0x} in terms of W_x . The coefficient and power of the derived N_{0x} - W_x relationships were averaged across the model output times examined in order to give a more general relation for each precipitating hydrometeor category. The plot showing an example of the dependence of N_{0r} on W_r from a single model time exhibits a high degree of scatter (Fig. 1.) However, the powers and coefficients of the derived relationship did not vary significantly across the range of times examined (not shown), which suggests confidence in the robustness of the derived relation.

The Milbrandt and Yau suite of microphysics 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_{ti} , is already diagnosed based upon temperature in the single-moment option, through Cooper’s equation (Cooper, 1986),

$$N_{ti} = 5 \exp (0.304 (273.15 - \max(233, T))), \quad (7)$$

where T is the temperature in Kelvin. For rain and the other three frozen categories, the number concentration is calculated as the zeroth moment of the distribution using the intercept parameter of the PSD of that species, which is set to a constant value for each species in the original single-moment microphysics scheme (see Table 1). The scatter plots showing the dependence of N_{0x} on W_x for snow, graupel and hail are shown in Figs. 2 through 4. The frozen hydrometeor concentrations are diagnosed based upon the water content within that hydrometeor category. The fixed N_0 values used in the original Milbrandt and Yau scheme and the fitted relation are also shown in the figures. Examining Figs. 1-4 and Table 1, it is clear that for each of the

hydrometeor species the coefficient differs significantly from the fixed value of N_{0x} , by up to three orders of magnitude in the case of graupel.

4. Numerical experiments

In order to test the diagnostic N_0 relations, several simulations of the May 3rd 1999 case were performed. The main aim of this study is to implement the diagnostic relations for N_{0x} within a single-moment microphysics scheme and determine how well such a single-moment scheme reproduces the results of double-moment scheme. Two baseline simulations are first produced, using the original MY1, MY2 schemes, respectively. The results of the diagnostic N_{0x} simulations are compared against these to gauge the impact and effectiveness of the diagnostic relations. Another simulation was performed using the original MY1 scheme with N_{0r} lowered from $8 \times 10^6 \text{ m}^{-4}$ to $4 \times 10^5 \text{ m}^{-4}$. Two further simulations were performed using the derived diagnostic N_{0x} relations, one in which only the warm rain processes used the diagnostic relation, and one in which the intercept parameters for both warm rain and ice processes, including 4 precipitating hydrometeors total, are diagnosed. Details of the simulations and the nomenclature used can be found in Table 2.

Each simulation was performed using the same model (ARPS) as the 250-m reference simulation that produced the synthetic dataset used for fitting the diagnostic relations. However, rather than the complex full physics real-data setup of the reference simulation, the simulations herein used the same single sounding and thermal bubble initialization procedure as in the idealized experiments of Dawson et al. (2010), and were performed at the same horizontal resolution of 500 m. 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 Dawson et al. (2010). The simulations *MY1_orig* and *MY2_orig* are identical to *MY1* and *MY2* from Dawson et al. (2010) and are repeated here mainly for convenience.

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 same as in the 250 m reference simulation. The fourth-order monotonic computational mixing scheme of Xue (2000) was utilized with a coefficient of 0.0015 s^{-1} . Each simulation used a different microphysical scheme setup, although all of these were based on either the MY1 or MY2 schemes (Milbrandt and Yau 2005b). 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, which was of horizontal dimensions 128 km $\times$ 175 km. 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 Dawson et al. (2010), and full details of the original real-data simulation can be found in Dawson et al. (2007).

5. Results and discussion

a. Reflectivity structure

The *MY1_orig* simulation produced a storm that did not show realistic mature supercell characteristics, as can be seen by the reflectivity structure (Fig. 5a). It must be noted that the storm in *MY1_orig* was beginning to decay by one hour into the simulation, due to the strong surging cold pool cutting off the updraft at the low levels in this simulation. The area of maximum surface reflectivity, located around 60 km from the western and 80 km from the

southern boundary of the domain, shows a maximum around 55 dBZ, although the lateral extent of the forward flank reflectivity region is smaller than we would expect for an event of this type.

The forward flank reflectivity region is more realistically represented in *MY2_orig* (Fig. 5b) than it is in the single-moment simulation, although in *MY2_orig* the forward flank reflectivity region is larger than expected. Morrison and Milbrandt (2011) found that the MY schemes produce long and narrow forward flank regions. This does not affect the key point of this paper since we are primarily interested in how well the results of the single-moment scheme can match the double-moment, as a proof-of-concept. The relative improvement in the forward flank reflectivity region in *MY2_orig* could be because the storm in *MY1_orig* decayed shortly after the time examined here, while the storm in *MY2_orig* correctly sustained. However, there are many processes that cannot be well represented within the single-moment scheme, such as size sorting. In contrast, the double-moment scheme does parameterize size sorting, although when the shape parameter α is set to 0 (as in *MY2_orig*), excessive size sorting tends to occur (Milbrandt and Yau 2005a). The effect of this excessive size sorting can be noted in Fig. 5b, in the sharp gradient at the leading edge of the forward flank reflectivity. Simulations of this case performed using the triple-moment Milbrandt and Yau microphysics scheme produced a more gradual and realistic reflectivity gradient in this region (see Fig. 3 in Dawson et al., 2010), corresponding more closely to radar observations of this case (Dawson et al. 2010).

MY1_N0, in which the rain intercept parameter value is reduced, is seen to produce a more realistic storm structure than *MY1_orig*, particularly on the leading edge or forward flank of the storm. The maximum reflectivity in this simulation is 61 dBZ, which is close to that of *MY2_orig*, and significantly increased from that of *MY1_orig*. Since the only difference between the two simulations is the reduction in the (fixed) value of N_{0r} , this would seem to indicate that

the default value of $8 \times 10^6 \text{ m}^{-4}$ for N_{0r} is too high for the type of severe convective case being simulated here, it will clearly not be optimized as the default Marshall-Palmer relation was derived for stratiform rain. For a given water content, increasing N_{0r} will decrease the median volume diameter, resulting in decreased reflectivity values. As was shown by Snook and Xue (2006), altering the intercept parameters for rain and hail PSDs can have a large impact on tornadogenesis, so we expect that reducing N_{0r} will result in significant changes in several fields. Despite the improved overall structure of the storm, the areal extent of the forward flank reflectivity region in *MY1_N0* is still significantly smaller compared to that in *MY2_orig*. The areal extent of reflectivity values greater than 30 dBZ is 110 km² in *MY1_orig*, 1072 km² in *MY2_orig* and 180 km² in *MY1_N0*. For a threshold value of 50 dBZ, the corresponding areas covered are 10 km², 52 km² and 43 km² respectively, illustrating the large forward flank region in *MY2_orig*.

The reflectivity structure produced by *diag_rain* is broadly similar to that of *MY1_N0*, although the lateral extent of the storm is slightly increased. The maximum reflectivity is similar to *MY1_N0* and *MY2_orig*. The forward flank region is better represented in *diag_rain* than in the fixed- N_{0r} experiments, with the strength of the east-west reflectivity gradient in the forward flank region being decreased in *diag_rain* (the reflectivity decreases to zero more gradually from west to east), which corresponds more closely to base reflectivity observations from KTLX (0.5° tilt, not shown). The area with reflectivity greater than 30 dBZ is 215 km² and that with greater than 50 dBZ is 54 km².

While diagnosing the intercept parameter of the rain PSD produces improvement over the original fixed- N_{0r} single-moment simulation, the improvement is mostly limited to the lowest levels, since the same ice phase processes are used in *diag_rain* as *MY1_orig*, and little

improvement is observed above the freezing level. At the surface, improvements in *diag_rain* in the forward flank region are still relatively small; it is hypothesized that this is because much of the liquid water in this region originates from melting and fallout from the anvil region, which is not well simulated by the fixed- N_0 experiments.

To investigate possible further improvements to the solution in the forward flank region, the diagnostic relations for the intercept parameters of snow, hail and graupel are implemented in *diag_all*. Examining the reflectivity structure generated by *diag_all*, (Fig. 5e) it is clear that the inclusion of diagnostic intercept parameters for graupel, snow and hail has a large effect on the lateral extent of the storm and general storm structure. The overall reflectivity structure is seen to resemble that of *MY2_orig* more closely than any other simulations. Particular improvement (again, “improvement” is defined relative to the *MY2_orig* simulation) is noticed in the forward flank region of the storm, with that of *diag_all* larger in size than in the other single-moment simulations. This increased areal extent in *diag_all* is mostly of reflectivity values below 30 dBZ, as the area covered with reflectivity of 30 dBZ is 205 km², which is lower than the corresponding area for *diag_rain*, although the area with reflectivity over 20 dBZ is greater for *diag_all* than *diag_rain*. This would suggest that by diagnosing the intercept parameters for the frozen categories, we are able to more accurately represent the ice processes that contribute to fall-out from the anvil. However, the maximum reflectivity seen in *diag_all* is reduced by around 10 dBZ from that of *MY2_orig*, to 43 dBZ, which is lower than we would expect for a storm of this nature. The lower reflectivity in *diag_all* than *diag_rain* is a consequence of a significant decrease in rain water mixing ratio seen in this simulation (Fig. 6). The maximum rain water mixing ratio at the surface in *diag_all* is 0.5 g kg⁻¹, over four times less than the maximum of 2.2 g kg⁻¹ in *diag_rain*. The horizontal-plane-maximum rain water mixing ratio in *diag_all* is less

than that in single-moment simulations at the 2 km height (Fig. 6) and it continues to decrease toward the surface. The cold pool in *diag_all* is much weaker than the other single-moment simulations (Fig. 8), resulting in more evaporation and decreased liquid rain water content, directly impacting the reflectivity.

Although it is expected that the greatest improvement will be seen at levels below the melting layer, the reflectivity structure is also examined at 5.5 km height. *MY1_N0* and *diag_rain* show little improvement over *MY1_orig* (Figs. 7a, 7c, 7d), which is expected as only the rain PSD is altered in these simulations. As at the surface, the forward flank reflectivity region is larger in extent in *MY2_orig* than the single-moment simulations (Fig. 7b), although the inclusion of the diagnostic relations for the frozen hydrometeors in *diag_all* (Fig. 7e) shows an increase in the areal extent of this region. We note here that the reflectivity calculation in each case is consistent with the DSD models used in each simulation.

b. Cold pool structure

The cold pool is discussed in terms of the equivalent potential temperature perturbation (θ_e') fields at the surface, as in Dawson et al (2010), since the θ_e' field also takes into account moisture effects. Here, θ_e is calculated according to Bolton (1980). According to Dawson et al. (2010), James and Markowski (2010) and McCaul and Cohen (2002), since θ_e is a conserved variable even in the presence of moist processes, θ_e can be used as an estimation for the source region of the air in the cold pool; below the level of minimum θ_e , lower values of θ_e indicate a higher source level of the surface air. Of course, the above statement assumes that θ_e is conserved in the downdraft, which is not strictly true. If turbulent mixing with the environment occurs, or any process that causes a departure from pseudoadiabatic descent (such as the melting of frozen hydrometeors) then θ_e will not be exactly conserved.

The cold pool produced in *MY1_orig* is seen to be very strong (Fig.8a). 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. This process is believed to be responsible for the mis-alignment of the low-level gust frontal forcing and the mid-level mesocyclone that causes the failure in tornadogenesis in Snook and Xue (2008). *MY1_orig* also produces a strong cold pool in the forward flank region of the storm, which was not observationally verified for this case. Mobile mesonet observations from May 3rd indicate that the cold pools in the forward flank region of the storm for this event were small and weak, with maximum temperature deficits of no more than 2-3 K (Markowski 2002). The maximum temperature deficit in *MY1_orig* is close to 8 K (not shown). The areal extent of the cold pool is examined through two metrics, the areas within which the θ_e deficit is greater than 5 K and 10 K. For *MY1_orig*, the areas are 680.5 km² and 451 km² for θ_e deficit exceeding 5 K and 10 K, respectively.

The cold pool in *MY2_orig* is very weak in comparison, with a maximum temperature deficit of 0.7 K (not shown), which is weaker than the cold pool observed by the mobile mesonet (Markowski 2002). The cold pool in the 250 m reference simulation is stronger than that seen in *MY2_orig*, and corresponds more closely to mobile mesonet observed temperature perturbations (Dawson 2009) which suggests that *MY2_orig* simulation at 3600s is producing a storm that is low-precipitation (LP) in character, as storm A was during its developing stage. The reduced strength of the cold pool in the forward flank region in *MY2_orig* as compared to *MY1_orig* also corresponds more closely to the mobile-mesonet-observed weak cold pool in this region (Markowski 2002). The maximum θ_e deficit is reduced to 18 K for *MY2_orig* from 30 K for *MY1_orig*, and the areas of 5 K and 10 K θ_e deficits decrease to 105 km² and 32 km² respectively.

The cold pool produced by *MYI_N0* is weaker than that of the original single-moment scheme, with a maximum temperature deficit of 4 K, a 5 K θ_e deficit covering 365 km² and a 10 K deficit covering 201 km². Snook and Xue (2008) 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 intercept parameter values. They concluded that this is due to distributions that favor fewer large drops (as characterized by a reduced intercept parameter) possessing a reduced total hydrometeor surface area when compared to the same mass of water distributed as a large number of smaller drops. This reduced surface area limits the potential for evaporative cooling, which is one of the most important mechanisms for cold pool formation. Ice processes also play an important role in cold pool formation, and this is discussed next.

The cold pool structure of *diag_rain* is intermediate between *MYI_orig* and *MYI_N0* in terms of both maximum strength and areal coverage. The cold pool produced by *diag_rain* is larger than that produced by *MYI_N0* (Figs. 8c, 8d). It seems that diagnosing N_{0r} does not improve the simulation in terms of the cold pool structure and intensity as much as simply reducing N_{0r} by a factor of 20; diagnostic treatment of the frozen hydrometeors may still be needed for more realistic simulation of the cold pool. While the cold pool in *MYI_N0* is weaker, we know the fixed N_{0r} value throughout the domain is not physically realistic.

The cold pool produced by *diag_all* that does include diagnostic treatment of ice PSDs is much weaker than the cold pool witnessed in any of the previous single-moment simulations. The maximum temperature deficit is 1.3 K (not shown), which is close to the maximum temperature deficit of 0.7 K in *MY2_orig*, and is closer to the observed cold pool intensity (Markowski 2002). The single-moment microphysics schemes, at least with their default

intercept parameter values, tend to produce unrealistically strong cold pools. This is partly due to the default values not necessarily being suitable for strong convective simulations. The diagnostic approach shows promise in producing more realistic cold pools without excessive intercept parameter tuning. The θ_e' field (Fig. 8e) for *diag_all* also shows a similar cold pool structure to that of *MY2_orig*, with the maximum θ_e deficit of -18.9 K (Fig. 8e) matching closely that of -18 K produced by *MY2_orig* and the areal extent of the 10 K θ_e deficit at 47 km² close to that of *MY2_orig* at 32 km². Although reducing the strength of the cold pool may not be desirable in all cases, the goal of this study is to recreate the key features of the double-moment scheme, which in this case presented with a cold pool of significantly reduced strength from the single-moment simulation.

c. Second moment of the distribution

The striking differences in storm structure and cold pool between *MY1_orig* and *MY1_N0* exemplify the large impact that PSD parameters can have upon the simulation results. Altering N_{0x} affects the simulation both directly through the impact on N_{tx} , and also indirectly through feedback from processes such as evaporative effects. The second moment (M_2) of the distribution is closely related to the surface area of the hydrometeors, and as such it is the most important moment for the evaporation rate. M_2 can be calculated using Eq. 3 and can be used to gain insight on the evaporation rate.

For each simulation, the average second moment was calculated for two thresholds; the average over all non-zero M_2 values in the simulation and the average over all points with reflectivity greater than 30 dBZ. The second threshold was used as both *MY2_orig* and *diag_all* have large regions of low reflectivity in the forward flank region, which will bias the average M_2

value. Across all non-zero valued points, the average value of M_2 for *MYI_orig* is $103.4 \text{ mm}^2 \text{ m}^{-3}$, for *MYI_N0* is $68.9 \text{ mm}^2 \text{ m}^{-3}$, and for *MY2_orig* is $25.7 \text{ mm}^2 \text{ m}^{-3}$. The corresponding values for *diag_rain* and *diag_all* are 1.61 and $0.95 \text{ mm}^2 \text{ m}^{-3}$, respectively. Clearly the large average M_2 in *MYI_orig* indicates a high evaporation rate, inducing the very strong cold pool in that simulation. Fig. 6 showed that *MYI_N0* and *diag_rain* had very similar horizontal-plane-maximum mixing ratio profiles, so the difference in average M_2 can be explained by consideration of the diagnostic relation for rain. The power in the relation is 0.566 , so for W of 0.041 g m^{-3} or below, a diagnosed N_0 would be decreased in *diag_rain* as compared to *MYI_N0*, and M_2 is proportional to N_0 . We expect less difference between the average M_2 values when only higher mixing ratio values are considered. The reflectivity threshold is used as a proxy for this. For areas over 30 dBZ , the average M_2 value for *MYI_orig* is $629.3 \text{ mm}^2 \text{ m}^{-3}$, for *MY2_orig* is $38.8 \text{ mm}^2 \text{ m}^{-3}$, and for *MYI_N0* is $230.9 \text{ mm}^2 \text{ m}^{-3}$. The average M_2 for *MYI_N0* quadruples when thresholded at 30 dBZ , but for *diag_rain* it increases almost tenfold from 1.61 to $15.1 \text{ mm}^2 \text{ m}^{-3}$. This is indicative of higher water content bringing the diagnosed N_0 closer in line with the fixed value. Thresholding at 30 dBZ increases the average M_2 of *diag_all* to $6.0 \text{ mm}^2 \text{ m}^{-3}$, a far lower increase than the fixed N_0 simulations, illustrating the reduced mixing ratio values in *diag_all* against the other simulations (also see Fig. 6).

We note here that even though similar results, in terms of the cold pool strength and precipitation structure, seem obtainable by choosing a smaller fixed value of the rain intercept parameter, in practice, it is difficult to predetermine what value should be used and the constant fixed values are not necessarily realistic. For this reason, we believe the diagnostic relations hold more promise; to say the least they provide spatial variability to the PSD parameters that appear to be more physical.

In terms of each of the variables examined in this study, consistent improvements are seen in *diag_rain* over *MY1_orig*. Further improvements in examined variables in *diag_all*, except for the weak reflectivity core, bring the results of that simulation further in line with results produced by the double-moment simulation, consistent with the goal of this study. This is encouraging, and it is suggested that the method of diagnosing the intercept parameters 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 double-moment results, we recognize that there is a limit to this approach; there are intrinsic limits to the single-moment scheme. The diagnostic relation for N_0 cannot fully represent all complex physical processes included in the double-moment scheme such as dynamic size sorting.

d. Evolution of surface RMS errors

As the goal of this study was to recreate the key features of the double-moment simulation through use of diagnostic relations for N_{0x} within the single-moment framework, the evolution of RMS errors in the surface temperature and θ_e fields is examined. As we seek to mimic the output of *MY2_orig*, RMS errors are calculated on the difference between the surface-level temperature and θ_e fields of *MY2_orig* and the four single-moment simulations.

The RMS errors in the temperature and θ_e fields indicate that throughout the simulation period, the cold pool in *diag_all* most closely matched that of *MY2_orig* (Fig. 9), while the cold pool in *MY1_N0* resembled the double-moment simulation more closely than that of *diag_rain*.

All of the simulations outperformed *MYI_orig*, with the RMS error in temperature of *MYI_orig* consistently double that of *MYI_N0* and 40% higher than *diag_rain* (Fig. 9). These results lend weight to the earlier assertion that diagnosing the intercept parameter for rain alone does not offer enough improvement in the cold pool over selecting a fixed, reduced (but arbitrary and perhaps tunable after the event) value for N_{0r} , and the form of the frozen hydrometeor distributions must also be considered in order to produce a more realistic cold pool intensity.

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 single-moment microphysics schemes in the hope of producing results closer to those of double-moment schemes. The PSD parameter chosen was the intercept parameter of the size distribution. 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 a realistic two-moment simulation. The original single-moment Milbrandt and Yau microphysics scheme uses a fixed value for the intercept parameter of the distribution of each hydrometeor species. Two control simulations were run using the original single and double-moment microphysics 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 showed improvements over *MYI_orig* in terms of producing results more closely aligned with those of the double-moment simulation (more realistic reflectivity structure, reduced cold pool strength, reduced number concentration.)

Diagnosing the intercept parameter of the rain PSD produced improvements upon the original fixed- N_{0r} single-moment simulation, however, these are limited to the lowest levels. The addition of a diagnostic relation for N_{0x} for the frozen hydrometeor categories is seen to have a greater impact on the simulation results than diagnosing N_{0r} only. Improvements are seen at low levels as well as above the melting layer, due to improvements in the structure of the frozen categories bringing improvements in the rain category through fallout and melting.

The use of diagnostic relations for several frozen species was seen to significantly increase the lateral extent of the storm in *diag_all* over the other single-moment simulations. Extending the diagnostic intercept parameter relation to the frozen hydrometeors also has a large positive impact on the cold pool structure. It is known that altering the intercept parameter 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 cooling (Snook and Xue, 2008, 2006; Gilmore et al., 2004).

While *diag_rain* produced a cold pool smaller in size and strength than that of *MY1_orig*, diagnosing the frozen category intercept parameters further reduced both the intensity and size of the cold pool, bringing the temperature deficit in line with that of *MY2_orig*. The cold pool in *MY2_orig* was seen to be very weak in the forward flank region, which agrees with surface mesonet observations from the event (Markowski 2002), hence improvements in the representation of the forward flank region through diagnosing the intercept parameters of the frozen species is encouraging.

While improvements are seen for the use of the diagnostic relations within these simulations, questions still exist about the representativeness of the derived $N_{0x} - W_x$ relations, especially in light of the significantly decreased reflectivity core in *diag_all*. This could be investigated

through the performance of simulations for a number of other cases. If the relations derived here are too case-specific, the inclusion of other cases into the study would allow us to derive a more general relation for each species. If relations are derived that diagnose N_{0x} for each of the precipitating hydrometeor species and are applicable to a range of different cases (for example severe convective storms, squall line cases, stratiform precipitation and winter storms), then this method shows considerable promise in improving the results of a six-prognostic-variable single-moment microphysics scheme, with considerably less increase in computational cost as compared to using a twelve-prognostic-variable double-moment scheme. It is hoped that through further exploration of the parameter space a set of relations can be derived that will be applicable to a range of situations. A further simulation was performed to investigate the specificity of the derived relations. The same model setup was used, with N_{0x} for each species diagnosed using the derived relations, but with the power in the diagnostic relations (see Table 1) set to 1 for each species. Results (not shown) were very similar to that of *diag_all*, which indicates that results seem to be not very sensitive to the exact value in the coefficient of the power law but further investigation is needed to ascertain this.

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Fig. 1. Dependence of rain intercept parameter (N_{0r}) on water content (W). Points are directly fitted using the zeroth and third moments of the exponential DSD to obtain the N_{0r} - W relation. The dashed line is the derived fitted relation (in linear space) and the bold line shows the fixed value of N_{0r} used in the original Milbrandt and Yau single-moment scheme.

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. Reflectivity and horizontal wind vectors at the surface (plotted every 2.5 km) at 3600 s into the five simulations: a) *MY1_orig*, b) *MY2_orig*, c) *MY1_N0*, d) *diag_rain* and e) *diag_all*.

Fig. 6. Horizontal-plane-maximum rain mixing ratio profiles at five levels in the lowest 2 km.

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Fig. 8. Surface equivalent potential temperature perturbation (shaded) and reflectivity (contours, 10 dBZ increment) for the five simulations as in Fig. 5.

Fig. 9. Evolution of the RMS error in equivalent potential temperature for each of the four single-moment simulations when compared to *MY2_orig*.

Table 1. The fixed N_{0x} values used in the original Milbrandt and Yau single-moment microphysics scheme, and the derived diagnostic relation for N_{0x} (based on W_x) for rain, snow, graupel and hail.

Species	Default fixed N_{0x} values	Diagnostic relation derived from real data simulation
Rain	$N_{0r} = 8 \times 10^6 \text{ m}^{-4}$	$N_{0r} = 2.45 \times 10^6 W_r^{0.566} \text{ m}^{-4}$
Snow	$N_{0s} = 3 \times 10^6 \text{ m}^{-4}$	$N_{0s} = 3.19 \times 10^9 W_s^{0.755} \text{ m}^{-4}$
Graupel	$N_{0g} = 4 \times 10^5 \text{ m}^{-4}$	$N_{0g} = 6.13 \times 10^8 W_g^{0.523} \text{ m}^{-4}$
Hail	$N_{0h} = 4 \times 10^4 \text{ m}^{-4}$	$N_{0h} = 5.13 \times 10^6 W_h^{0.467} \text{ m}^{-4}$

Table 2. Description of the microphysical setup used in the five simulations that were performed at 500m horizontal resolution.

Experiment Name	Details of microphysics scheme
<i>MY1 orig</i>	Original single-moment Milbrandt and Yau scheme.
<i>MY2 orig</i>	Original double-moment Milbrandt and Yau scheme.
<i>MY1 N0</i>	Single-moment with reduced fixed value of $N_{0r} = 4 \times 10^5 \text{ m}^{-4}$.
<i>diag rain</i>	Single-moment with intercept parameter diagnosed for rain only.
<i>diag_all</i>	Single-moment with intercept parameter diagnosed for all precipitating hydrometeor categories.

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Fig. 8. Surface equivalent potential temperature perturbation (shaded) and reflectivity (contours, 10 dBZ increment) for the five simulations as in Fig. 5.

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811 Fig. 9. Evolution of the RMS error in equivalent potential temperature for each of the four
 812 single-moment simulations when compared to *MY2_orig*.

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