Sedimentation-Induced Errors in Bulk Microphysics Schemes

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ABSTRACT

The computation of hydrometeor sedimentation in one-moment, two-moment, and three-moment bulk microphysics parameterizations is examined in the context of a 1D model, with no other microphysical processes active. The solution from an analytic bin model is used as a reference against which the bulk model simulations are compared. Errors in the computed (nonprognostic) moments from 0 to 7 from the bulk model runs are examined. In addition to the commonly used predicted variables (number concentration, mass, and reflectivity), bulk scheme configurations with alternative combinations of prognostic moments are considered.

While the extra degree of freedom in a two-moment scheme adds realism to the simulation of sedimentation over a one-moment scheme, the standard practice of imposing a constant relative dispersion in the particle size distribution results in considerable errors in some of the computed moments. The error can be shifted to different moments by selecting different prognostic moments. For three-moment schemes, the error is considerably reduced over a wide range of computed moments and there is much less sensitivity to the choice of prognostic variables.

Two alternative approaches are proposed for modifying the computation of sedimentation in two-moment schemes to reduce problems associated with excess size sorting. The first approach uses a diagnostic relative dispersion (shape) parameter, generalized for any pair of prognostic moments. The second involves progressively reducing the differential fall velocities between the moments and is therefore applicable for schemes that hold the shape parameter constant. Both approaches greatly reduce the errors in the computed moments, including those on which microphysical process rates depend, and are easily applied to existing two-moment schemes.

1. Introduction

In 3D atmospheric models that are run at the convective scale, the effects of cloud microphysical processes are generally computed by a bulk microphysics scheme (BMS). In a BMS, the particle size distribution (PSD) of each hydrometeor category is approximated by a continuous function for which there are one or more free parameters. Correspondingly, there are one or more prognostic moments of the distribution, for which predictive equations for microphysical processes and sedimentation are computed. In part because of computational constraints, nearly all of the early schemes predicted only a single moment of the PSD, the third moment with respect to diameter, which is proportional to the hydrometeor mass content \(^1\) (e.g., Kessler 1969; Rutledge and Hobbs 1983; Lin et al. 1983; Walko et al. 1995; Thompson et al. 2004). Recently, two-moment schemes have become more widely used (e.g., Murakami 1990; Ferrier 1994; Reisner et al. 1998; Seifert and Beheng 2001; Morrison et al. 2005; Milbrandt and Yau 2005b). These schemes generally predict the zeroth moment (equal to the total number concentration \(N_T\)) and the third moment, although there is no intrinsic requirement for the choice of prognostic variables. Milbrandt and Yau (2005a, hereafter MY05a) and Milbrandt and Yau 2005b extended the bulk approach to include a prognostic equation for the sixth moment, radar reflectivity, for a three-moment BMS. Despite the increasing use of

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\(^1\) This is true for hydrometeor categories with fixed bulk densities, where the exponent in the mass–diameter relation equals 3. However, for categories such as snow, where an exponent of 2 is often used, it is the second moment that is prognostic.
BMSs in research and in operational numerical weather prediction, there has been very little attention paid to the consideration of using other prognostic moments.

Some examination of the treatment of sedimentation in BMSs has been reported in the last decade. Wacker and Seifert (2001, hereafter WS01) investigated the differences in vertical profiles of LWC resulting from the sedimentation of rain between a spectral model, taken as the reference solution, and one- and two-moment bulk model solutions, starting with an idealized profile. The budget equations for the prognostic moments in the bulk models were solved analytically in the form of quasilinear advection equations. The resulting solutions exhibited shock wave features. These were interpreted as artifacts of the numerical method and generally do not appear in atmospheric models, whose computation of sedimentation is usually performed with diffusive numerical algorithms. The two-moment scheme, while producing a solution closer to the reference solution than the one-moment scheme, suffered from excessively large sedimentation rates. Two limitations of this study pertaining to the bulk model solutions were the use of a single set of prognostic moments and the constraint of an inverse-exponential PSD.

Using an approach similar to that of WS01, MY05a further examined bulk model sedimentation, comparing profiles of bulk model calculations of pure sedimentation to a spectral reference solution. It was shown that while in a one-moment scheme all quantities are simply single-value functions of the prognostic moment, a two-moment scheme can mimic the effects of gravitational size sorting, whereby the mean particle diameter increases with decreasing height during the simulation. This results directly from the use of moment-weighted fall velocities for the sedimentation rates of each moment. When the PSD is constrained to an inverse-exponential function, this differential sedimentation leads to excessive size sorting in a two-moment scheme, accounting for some of the problems in the two-moment results of WS01. MY05a relaxed the restriction of an inverse-exponential distribution and used a three-parameter gamma distribution function of the form

$$N(D) = n_0 D^\mu e^{-\lambda D}, \quad (1)$$

where $n_0$, $\mu$, and $\lambda$ are referred to as the intercept, shape, and slope parameters, respectively, and (1) reduces to an inverse-exponential distribution for $\mu = 0$. In addition to testing other fixed values of $\mu$, the effects of allowing this parameter to vary in time during the simulations were considered. This was done using two approaches: the first used a two-moment approach with $\mu$ treated as a diagnostic function of the prognostic moments, and the second used a three-moment approach, whereby $\mu$ was a free parameter. The solutions demonstrated that by allowing the shape parameter to vary, either diagnostically or prognostically, the problems associated with excessive size sorting are controllable. MY05a limited their considerations to the “standard” combinations of prognostic moments, $M_3, M_0-M_3$, and $M_2-M_3-M_6$ for the one-, two-, and three-moment bulk scheme calculations, respectively, where $M_k$ is the $k$th moment of (1).

Using an experimental framework similar to these earlier studies, Wacker and Lüpkes (2009, hereafter WL09) were the first to begin to examine the effects of using other prognostic moments for bulk model calculations of pure sedimentation. They showed that changing the prognostic moments affects the prediction of the profiles of $N_T$, LWC, and reflectivity and that there is considerable nonconservation of moments that are far from the order of the prognostic moments, which are the only conserved quantities. The computed values of moments between the prognostic moments were found to be underpredicted compared to the reference solution. In contrast, there was an overprediction of the moments outside of the range of predicted moments—lower (higher) than the lowest (highest) prognostic moment. Based on this, it was recommended that the order of the prognostic moments be chosen to be as close as possible to those that have the greatest effect on the evolution of the simulation. WL09 provide a strong motivation for further examination of the impact of the choice of prognostic moments in bulk schemes. Their study, however, was limited to one-moment and two-moment schemes and examined only two-moment schemes with fixed values of $\mu$.

The importance of a variable shape parameter and the added value of a third prognostic moment (MY05a) and the sensitivity to the choice of prognostic moments (WL09) are the bases of the motivation of this study. To date, there has been no comprehensive study on the impact of the selection of prognostic moments in two-moment bulk schemes with variable shape parameters or in three-moment schemes. It is the objective of this paper to examine these points in some detail. The ultimate goal of this study is to quantify the sedimentation-induced errors associated with a given selection of prognostic and diagnostic variables in order to guide cloud modelers as to the selection of prognostic moments in BMSs.

The paper is organized as follows. Section 2 describes the experimental design and the approach used to evaluate the different bulk model simulations. Section 3 provides a summary of the bulk results using different combinations of prognostic moments and presents an
analysis of the errors. Section 4 discusses two alternatives to controlling excessive size sorting in the fixed-\(\mu\) two-moment approach. Concluding remarks are given in section 5.

2. Experimental setup

a. Bin model

The experimental framework for this study is designed to investigate errors associated with pure sedimentation. No other microphysical processes are considered. Analytic results from a spectral model are used as the reference solution against which bulk model solutions are evaluated. We have employed a set of initial conditions that are nearly identical to those of WL09 to facilitate comparisons between the studies. An initial 1.5-km-deep square wave profile of rain is used, with an LWC of \(0.5 \times 10^{-3}\) kg m\(^{-3}\) and an \(N_T\) of \(3 \times 10^3\) m\(^{-3}\), with an inverse-exponential PSD [given by (1) with \(\mu = 0\)]. This \(N_T\) is equivalent to prescribing an initial intercept parameter \(n_0 = 8 \times 10^6\) m\(^{-4}\). The only difference between the initialization of this experiment and that of WL09 is that the rain in our initial profile is located higher, between 6500 and 8000 m above the surface rather than between 2500 and 4000 m. We choose to locate the initial rain at this higher altitude because the results presented can apply to any hydrometeor category, including hail, that can exist throughout a very deep atmospheric layer. Furthermore, although rain does not typically exist up to 8000 m, rain in a convective cloud may fall through a weak updraft and hence actually travel a much greater distance relative to the air than the distance from height it originates to the ground. Thus, the evolution of the model profiles over a deep column is of interest.

The computation of the analytic solution using the bin model is described in appendix A. The reference solution at various times for vertical profiles of \(M_0\) (\(N_T\)), \(M_3\) (proportional to LWC), \(M_6\) (reflectivity), and the mean-mass diameter \(D_m\) are shown in Fig. 1, where LWC is related to \(M_3\) by

\[
\text{LWC} = \frac{6}{\pi \rho_L} M_3, \tag{2}
\]

where \(\rho_L\) is the density of liquid water, and

\[
D_m = \bigg(\frac{6 \text{LWC}}{\pi \rho_L N_T}\bigg)^{1/3}. \tag{3}
\]

From (2) and (3), \(D_m = (M_3/M_0)^{1/3}\) since \(N_T = M_0\). Note that the reference solution profiles shown in Fig. 1 are displaced vertically as noted above but otherwise are identical to those of WL09 for their \(\mu = 0\) calculations (their Fig. 2, top panels). It is evident from Fig. 1 that the peak values of each moment sediment faster the higher the moment and the peaks for all moments decrease in time. The effects of size sorting are clearly evident from the profiles of \(D_m\) (Fig. 1d), which show that after a given time, starting from an initial distribution of equal sized particles, the mean-particle size increases with decreasing altitude since the largest and hence fastest-falling drops arrive first at the lowest levels.
b. Bulk model

The bulk model simulations are initialized with the same profile as the spectral model. The initial values of $M_0$, $M_3$, $\mu$, and $n_0$ are prescribed, with $\lambda$ computed from (B1). The PSDs for the bulk models are constrained by (1) at all times. With the three distribution parameters, the value of any moment $M_k$ can be computed analytically from

$$M_k = \int_0^\infty D^k N(D) \, dD = n_0 \Gamma(k + \mu + 1) \lambda^{-(k+\mu+1)}, \quad (4)$$

where $\Gamma$ is the gamma function. The evolutions of one, two, or three prognostic moments during sedimentation are solved using the prognostic equation for the given moment, derived from the budget equation for the size distribution:

$$\frac{\partial M_k}{\partial t} - \frac{\partial F_k}{\partial z} = 0, \quad (5)$$

where $F_k$ is the flux of $M_k$, given by

$$F_k = \int_0^\infty V(D) D^k N(D) \, dD, \quad (6)$$

with $V(D)$ given by (A1). Equation (5) can be written as

$$\frac{\partial M_k}{\partial t} - \frac{\partial (M_k V_k)}{\partial z} = 0, \quad (7)$$

where $V_k$ is the $k$th moment weighted sedimentation velocity, given by

$$V_k = \gamma a \frac{\Gamma(1 + k + \mu + b)}{\Gamma(1 + k + \mu + b)} \lambda^{-b}. \quad (8)$$

A discretized version of (7) is then solved numerically using the box-Lagrangian advection scheme (Kato 1995). However, in this study the Courant number was always less than one, for which case the box-Lagrangian scheme produces identical results to an Euler-forward scheme.

At each time step, the PSD parameters are first determined from the prognostic moments and/or closure assumptions for the given bulk scheme, the sedimentation velocities are calculated, and then (7) is solved for one step to compute the updated values of the prognostic moments. For all of the one-moment simulations in this study, the closure assumptions are $n_0 = 8 \times 10^6 \, m^{-4}$ and $\mu = 0$ at all times (as in WL09), with $\lambda$ computed from (B1). For the two-moment runs discussed in section 3, the only constraint is a constant $\mu = 0$. Equations (B1) and (B2) are used to determine $\lambda$ and $n_0$, respectively. In section 4, two-moment runs with alternative treatments of $\mu$ are examined. For the three-moment model, no closure assumptions are required since there are as many prognostic moments as there are PSD parameters in (1). For the initial time, the value of the third prognostic moment is computed from (B3). At each subsequent time step, (B1), (B2), and (B3) are used to compute $\lambda$, $n_0$, and $\mu$, respectively.

A series of bulk model simulations are performed, all starting with the same initial conditions and integrated for 2000 s. In each of the simulations, the choices of prognostic moments and/or closure assumptions are varied. To limit the number of runs, only integer moments between $M_0$ and $M_5$ are considered, although any positive real-valued prognostic moment is possible. We remark that there are qualitative differences in the bulk model solutions of MY05a and WL09, beyond differences due to different initial conditions and fall velocity parameters. In particular, the solutions of MY05a are much more diffusive (e.g., compare Fig. 3 in MY05a and Fig. 4 in WL09). This is due to the use of a relatively coarser grid spacing (~150 m) in the simulations of MY05a, and thus a smaller sedimentation Courant number, although this does not affect any of the conclusions drawn. In this study, the bulk model uses a vertical grid spacing of 12.5 m and a time step of 0.25 s.

c. Description of evaluation method

To provide guidance for the choice of prognostic moment, it is necessary to evaluate the ability of bulk schemes with different configurations to simulate the evolution of various moments that are deemed important (which are not necessarily the prognostic ones). The importance of any given moment depends entirely on the application. For the pure sedimentation of moment $M_k$, the sedimentation flux depends on $M_{k+b}$ [through (7) and (8)]. In a full BMS, the majority of mass transfer between water species results from accretion and diffusional growth/decay. It can be readily shown from the microphysical equations that the collection rate for a given hydrometeor is strongly dependent on moments $M_{2+b}$, $M_{1+b}$, and $M_b$ (including ventilation effects; e.g., Milbrandt and Yau 2005b), all of which can be computed from (4) upon first computing the size distribution parameters from the prognostic moments of the given scheme, as described in appendix B. Similarly, the diffusional growth rate is dependent on $M_1$ and $M_{1.5+b}$. Therefore, errors in these computed moments translate directly into errors in the instantaneous process rates on which they depend. For example, the continuous collection of cloud water by hail depends directly on $M_{2.6+b}$ with $b = 0.6$ for hail (e.g., Milbrandt and Yau 2005b). Thus, an error of 20% too great for the computation
of $M_{2.6}$ implies an overestimation of 20% for the instantaneous accretional growth rate of hail. Another important quantity in some BMSs is $D_m$, which is given by (3) and is therefore proportional to the ratio of $M_3/M_0$. The moment $M_6$ (reflectivity) is important if radar reflectivity data are assimilated into the model and is useful for model verification against radar observations. If a given moment is of no practical interest, then errors in its prediction are essentially unimportant.

Because of the large number of moments of potential interest, the errors in the profiles of a range of moments for a given bulk model simulation at a given time are presented in the form of 2D error plots (Fig. 2). In this example, the plot summarizes both the results and the errors for a particular bulk model simulation using a one-moment scheme with $M_3$ as the prognostic moment (discussed in the following section) at an integration time of 600 s. The profiles for $M_0$, $M_3$, and $M_6$, projected from the page, denote the respective instantaneous profiles from the reference solution (pink, as in the profiles in Fig. 1 but normalized by the initial peak value in the reference model for the given moment and projected onto the 2D plot as black contours), the bulk model (green, as in the profiles in Fig. 3, but normalized), and the error (blue dashed), which is the field projected onto the 2D plot as colors. The color shading therefore summarizes the relative error from the bulk scheme for a range of moments from $M_0$ to $M_7$, while contours denote the moment values from the bulk solution, normalized by their initial values. It can be readily seen which moments, and at which altitudes, are overpredicted (underpredicted) with respect to the reference solution as indicated by the warm (cold) colors in the error plots. These plots are used in the following sections for the comparison of different bulk model configurations.

Simple metrics to rank the overall skill of the various bulk schemes are also desirable, given the infinite number of possible combinations of prognostic moments for multimoment schemes. Depending on which moments are deemed important for a given application, different metrics should be used. Here, the time-averaged (for 2000 s, the total simulation time) normalized mean absolute errors (NMAEs) are computed, with equal weight given to each of $M_0$–$M_7$, $M_0$–$M_3$, and the prognostic
moments for a given run. This metric is designed to include weight from all moments that could be important, up to (and slightly beyond) \( M_6 \) for reflectivity, with extra weight placed on the moments that are important for the microphysical growth rates (\( M_0-M_3 \)), plus the prognostic moments themselves. This metric will be used to provide a ranked list of bulk model configurations (i.e., with a combination of prognostic moments), discussed below.

3. Results and error analysis

The results from bulk model calculations from several combinations of prognostic moments are examined. In this section, we first look at the sedimentation profiles and error plots from the most commonly used configurations of one-, two-, and three-moment schemes and then proceed to inspect the error plots for several alternative bulk configurations.

a. Commonly used bulk configurations

Figure 3 depicts vertical profiles, corresponding to those of the spectral reference solution (Fig. 1), for a one-moment scheme with a prognostic \( M_3 \) and a constant \( n_0 = 8 \times 10^6 \text{ m}^{-4} \) and \( \mu = 0 \). The pattern of LWC (\( M_3 \); Fig. 3b) essentially translates downward at a constant sedimentation velocity, with smoothing due to the numerical method, particularly at the trailing edge. The other moments (\( M_0 \) and \( M_6 \); Figs. 3a,c) are monotonically related to \( M_3 \). Because of the single degree of freedom, one-moment schemes are incapable of producing any size sorting effects due to pure sedimentation, as is evident in Fig. 3d. The corresponding error plots are shown in Fig. 4 for various times. It can be readily seen that values for all diagnostic moments within the range shown in the plots are overpredicted in the one-moment scheme at levels near the peak value in the bulk model. Similarly, the values ahead of (below) and behind (above) the peak are generally underpredicted compared to the reference solution, except for moments higher than \( M_4 \) in the regions trailing the peaks.

Since two-moment BMSs generally predict \( M_0 \) and \( M_3 \)—allowing \( n_0 \) and \( \lambda \) to vary diagnostically but maintaining a constant \( \mu = 0 \)—this configuration is examined. The resulting profiles (Fig. 5) are notably different from those of the one-moment prognostic \( M_3 \) scheme (Fig. 3). Clearly, \( M_6 \) is not related as a single-valued function of either of the two prognostic moments. The two-moment solution is somewhat closer to the reference solution (Fig. 1) in that the peaks of \( M_0 \) and \( M_3 \) decrease in time and \( M_3 \) sediments faster than \( M_0 \). Furthermore, of particular importance is the fact that the two-moment scheme produces a size-sorting effect, evident in the \( D_m \) profiles (Fig. 5d). However, this particular two-moment configuration clearly suffers from excessive size sorting when compared to the reference solution (Fig. 1d). This is related to the excessively large sedimentation rate of \( M_3 \) (Fig. 5b), which is due to the treatment of \( \mu \) (discussed in section 4). The error plots

\[ \text{Fig. 3. As in Fig. 1, but for a bulk model solution, one-moment, prognostic-} M_3, \mu = 0 \text{ configuration.} \]
for this run (Fig. 6) indicate that this problem manifests in the form of very large overprediction of moments higher than $M_3$, which is the highest prognostic moment, and underprediction of the lower moments. The behavior of two-moment schemes with other prognostic moments is discussed below, and alternative approaches to controlling the size sorting in a prognostic $M_0$-$M_3$ scheme are examined in section 4.

Sedimentation profiles and error plots from a three-moment prognostic $M_0$-$M_3$-$M_6$ scheme are shown in Figs. 7 and 8, respectively. To date, this is the only combination of prognostic moments that has been used for 3D atmospheric simulations using a full three-moment BMS (Milbrandt and Yau 2006a; Milbrandt et al. 2008; Dawson et al. 2010). While qualitatively similar to the two-moment results discussed above for lower-order moments, the three-moment scheme shows a fundamental improvement. Size sorting is essentially controlled (Fig. 7e); although the maximum $D_m$ from the three-moment run is larger at $t = 300$ s compared to that of the reference model.

**Fig. 4.** Error plots for a simulation using a one-moment scheme, prognostic-$M_3$, $\mu = 0$ configuration, at simulation times (a) 0, (b) 400, (c) 800, (d) 1200, and (e) 1600 s.

**Fig. 5.** As in Fig. 1, but for a bulk model solution, two-moment, prognostic $M_0$-$M_3$, $\mu = 0$ configuration.
Errors in Computed Moments: 2-Moment, $M_0-\mu = 0$ configuration.

(Fig. 1d), which is prescribed to have a maximum value of 0.010 m (appendix A). $D_m$ does not become extremely large as in the two-moment run (Fig. 5d), and the three-moment $D_m$ profiles generally match those of the reference model quite closely. The resulting profiles of the prognostic moments (Figs. 7a–c) are now very similar to the reference profiles (Figs. 1a–c). The errors for all of the moments between $M_0$ and $M_7$ (Fig. 8) are greatly reduced compared to those of both the one-moment ($M_3$) and two-moment ($M_0-M_3; \mu = 0$) results (Figs. 4 and 6, respectively).

b. Alternative combinations of prognostic moments

It is not clear that the traditional moment selection described in the previous section minimizes sedimentation-induced errors. Their usage in BMSs stems from the fact that microphysical source/sink terms are readily formulated for $N_T$ ($M_0$) and mass ($M_3$). However, any moment can be diagnosed from the predicted parameters and closure assumptions of the model by (4). This implies that any BMS could, in principle, use traditional moments for the physical source/sink term calculations while

Moment Profiles for Bulk Model: 3-Moment, $M_0-\mu = 0$, $M_6$

Fig. 7. As in Fig. 1, but for a bulk model solution, three-moment, prognostic $M_0-M_3-M_6$, configuration.
employing a different set of moments for sedimentation. This would allow model developers to select the best set of moments for a particular application within the BMS. To provide a basis for such a selection for sedimentation, the errors associated with combinations of prognostic moments other than the configurations generally used in 3D models are examined. Figures 9–11 depict the error plots for bulk model sedimentation calculations at 600 s for various combinations of one-, two-, and three-moment schemes, respectively. The moment errors at this particular time adequately summarize the general behavior of the models.

For the one-moment schemes, simulations with all integral moments from $M_0$ to $M_9$ were performed. The error plots for the runs with $M_0$, $M_3$, and $M_6$ as the prognostic moment are shown in Fig. 9. The vertical profiles are qualitatively similar to those of the prognostic $M_3$ run (Fig. 3), but with the translation speed systematically slower (faster) for lower (higher)-order prognostic moments. This is indicated in the error plots (Fig. 9), all of which are all qualitatively similar to those of $M_3$ (Fig. 4), but the more the region of overprediction is shifted upward (downward), the lower (higher) is the number of the prognostic moment.

For two-moment schemes, simulations using all combinations of integral prognostic moments between $M_0$ and $M_9$ were conducted, all with constant $m_5$ as above. The error plots shown in Fig. 10 comprise a subset of the results that is sufficient to illustrate the variation of the observed errors. In general, the values of diagnostic moments between the prognostic moments are underpredicted. The severity of this error increases

**Errors in Computed Moments: 3-Moment, $M_0$-$M_3$-$M_6$**

![Fig. 8](image)

**Fig. 8.** As in Fig. 4, but for a three-moment scheme, prognostic $M_0$-$M_3$-$M_6$ configuration.

**Errors in Computed Moments for 1-Moment schemes (600 s)**

![Fig. 9](image)

**Fig. 9.** Error plots at simulation time 600 s for various one-moment schemes. The prognostic moment for each configuration is indicated in the panels. For all runs, $\mu = 0$. 

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with the distance between the prognostic moments. For example, there is a similar underprediction of the moments between $M_0$ and $M_2$ for the $M_0$-$M_2$ combination (Fig. 10a), between $M_3$ and $M_5$ for the $M_3$-$M_5$ combination (Fig. 10b), and between $M_6$ and $M_8$ for the $M_6$-$M_8$ combination (Fig. 10c), all of which have prognostic moments that differ in number by 2. The underprediction is larger for moments between the prognostic ones for the runs where the prognostic moment numbers differ by 3 ($M_0$-$M_3$, Fig. 10d; $M_3$-$M_6$, Fig. 10e; and $M_6$-$M_9$, Fig. 10f), even larger when they differ by 4 ($M_0$-$M_4$, Fig. 10g; $M_4$-$M_8$, Fig. 10h), and largest for the $M_0$-$M_8$ combination (Fig. 10i). In all cases, the diagnostic moments outside of the range of prognostic moments—either lower than the lowest prognostic moment or higher than the highest—are greatly overpredicted. WL09 refer to this behavior as an “overshooting” of the diagnostic moment and explain that this problem results directly from the fact that for $j < k$ the prognostic moment $M_k$ sediments faster than $M_j$, which results in large values of a diagnostic $M_l$ according to (B8) in WL09, which shows that $M_l \propto (M_j^{k-1}/M_k^{j-1})^{1/(k-j)}$. Thus, there is overshooting for all moments $M_l$ for $l < j, k$ whenever $M_k$ becomes very small (at high altitudes) or for $l > j, k$ whenever $M_j$ is small (at low altitudes).

A large number of three-moment schemes simulations were performed with various combinations of integral moments. The error plots for a selection of the runs are shown in Fig. 11. There is no problem with large systematic overprediction for moments outside of the prognostic moments. This is because $\mu$ is not a constant parameter in a three-moment scheme, which implies that the speed of the prognostic moments relative to each other, and thus the rate of size sorting, changes in time. This is a desirable effect of the variable shape parameter and is discussed further in section 4. For configurations with prognostic moment numbers separated by 1 ($M_0$-$M_1$-$M_2$, Fig. 11a; $M_3$-$M_4$-$M_5$, Fig. 11b; and $M_7$-$M_8$-$M_9$, Fig. 11c), there is a general underprediction for the nonprognostic moments. For all of the three-moment simulations with the prognostic moment numbers separated by two or more, the errors are
Errors in Computed Moments for 3-Moment schemes (600 s)

Fig. 11. As in Fig. 9, but for various three-moment schemes.

generally quite low compared to the one- and two-moment runs. There is no clear trend in the errors for these three-moment runs, except for a tendency of underprediction of the moments lower than the lowest prognostic moment (e.g., Figs. 11e,f,h,i). For some combinations where the lowest prognostic moment is higher than \( M_0 \) (e.g., Figs. 11c,f,i), as well as runs not shown in Fig. 11, there is a pronounced overprediction of moments near \( M_0 \) at high altitudes.

c. Discussion of error scores

For each of the simulations undertaken in this study, an error score is computed based on the metric described in section 2. The scheme configurations and their corresponding error scores are listed in Table 1 in order of increasing score (decreasing skill). The three-moment runs generally, though not for all moment combinations, have the least amount of error, with the \( M_1-M_3-M_5 \) configuration scoring the best (lowest). The “standard” prognostic \( M_0-M_3-M_6 \) configuration, while having a relatively good error score compared to many of the other bulk schemes considered, ranks more poorly than several of the alternative three-moment configurations, demonstrating that a careful selection of the moments used for sedimentation may yield improvements even in three-moment BMSs. This indicates that the overall simulation skill for a three-moment scheme can be improved by alternate choices of prognostic moments, provided that microphysical process rates can be properly formulated for these moments.

The error score for the standard two-moment configuration (prognostic \( M_0-M_3 \), with \( \mu = 0 \)) is very large, being worse than all but one of the other bulk schemes discussed, including the standard one-moment configuration (\( M_3; \mu = 0 \)). This poor performance is largely due to uncontrolled size sorting and the associated overprediction of higher-order moments. Since the metric incorporates errors in these moments (i.e., between \( M_3 \) and \( M_7 \)), the metric scores of schemes with this error mode are degraded. For modeling applications that are not concerned with errors in the higher moments, a different metric may be more appropriate and this
two-moment configuration may not be as poor as suggested by Table 1. Nevertheless, it is generally desirable to have a bulk scheme that minimizes sedimentation-induced errors for a large range of computed moments. Thus, the large errors in the most commonly used two-moment scheme configuration indicate either that different prognostic moments should be used or that a method to control the deleterious effects of excessive size sorting should be considered.

4. Controlling size sorting in a two-moment scheme

a. Background of the problem

It may appear from the results presented in section 3 that the overshooting problems associated with two-moment schemes represent a severe detriment that may be insufficiently compensated by the ability to simulate the effects of size sorting and that a three-moment approach is the only robust method to properly modeling sedimentation. However, the results presented in section 3 were limited to two-moment schemes with a constant $\mu = 0$. MY05a showed that by diagnosing $\mu$ as a monotonically increasing diagnostic function of $D_m$, a prognostic $M_0-M_3$ two-moment scheme can in fact closely reproduce a prognostic $M_0-M_3$ three-moment scheme for pure sedimentation, with size sorting essentially controlled. In this section, the diagnostic-$\mu$ approach is generalized for other two-moment schemes. We also propose an alternative approach for controlling size sorting for two-moment schemes that are constrained to hold $\mu$ constant.

To understand why excessive size sorting occurs and how it can be controlled, consider the ratio between the moment-weighted sedimentation velocities, each given by (8), for the two prognostic moments $j$ and $k$ (where $j < k$) in a two-moment scheme:

$$
\frac{V_k}{V_j} = \frac{\Gamma(k + 1 + \mu + b)\Gamma(j + 1 + \mu)}{\Gamma(j + 1 + \mu + b)\Gamma(k + 1 + \mu)}.
$$

This ratio is plotted against $\mu$ for different $j, k$ pairs in Fig. 12. For a given constant value of $\mu \geq 0$, $V_k/V_j$ has a constant positive value $>1$. Thus, the sedimentation rate of $M_k$ is always greater than that of $M_j$, as is apparent from profiles shown in Fig. 5, for the case of $j = 0$ and $k = 3$. From (3) it can be deduced that at the leading (lower) edge of a profile of sedimenting hydrometeors $D_m$ will constantly increase because of the constantly increasing ratio $M_j/M_0$, in the framework of pure sedimentation. This behavior is a direct result of the constraint of a constant $\mu$ and thus an implicitly prescribed value of the ratio of the bulk fall velocities (Fig. 12). MY05a and WL09 showed that the problem

![Fig. 12](https://example.com/fig12.png)
can be mitigated somewhat by using a higher fixed value of $m$, which has the effect of making the bulk fall velocities closer in value, according to (9). An alternative would be to artificially bring $V_k/V_j$ closer to unity, by simply adding a factor to the computation of $V_j$, for example, without actually changing $m$. These approaches mitigate the problem but they do not eliminate it since with $V_k/V_j > 1$, the ratio of $M_3/M_0$—and hence $D_m$—will always increase in time at the leading edge due to sedimentation.

b. Diagnostic-$\mu$ approach

It was shown in MY05a that a diagnostic relationship for $\mu = f(D_m)$ is sufficient to narrow the PSD in a two-moment scheme, thereby controlling the size sorting. This is physically consistent with the mean sizes for a population of particles becoming large, and $V_k/V_j$ tends toward unity, consequently controlling the excessive size sorting that occurs if $\mu$ is held constant. The MY05a parameterization of $\mu = f(D_m)$ breaks down at the upper levels of a profile, where the mean sizes are small but the size distribution need not be broad. Furthermore, it was designed specifically for an $M_0-M_3$ scheme and hence may not necessarily work well if other prognostic moments are chosen.

The diagnostic $\mu$ approach can be generalized for any pair of prognostic moments by using the sedimentation profiles from the reference solution, from which the value of any moment can be computed at any level or time by (A3). By fitting the PSD to a gamma function of the form of (1), the value of $\mu$ can be solved for in the same method as described above for a three-moment scheme (see appendix B), using three arbitrarily chosen moments. The resulting profiles of $\mu$ at various times, computed using different combinations of three moments $i$, $j$, and $k$, are shown in the top panels of Fig. 13. Since the PSDs from the reference solution are not gamma functions (except at the initial time), the value of $\mu$ obtained from fitting the distributions to (1) depends on the choice of moments (which range from 0 to 6);
hence, there is some spread in the curves for the different \(i-j-k\) combinations. The bottom panels in Fig. 13 show the corresponding profiles of \((M_i/M_j)^{(k-j)}\), which is the ratio of the first two moments used for the fit to a gamma function, converted to units of meters. Although there is some spread at the higher levels where the total number of particles remaining is relatively low (see Fig. 1), this quantity is relatively independent of the choice of moments.

The similarity in the behavior of the two sets of profiles motivates the parameterization of \(\mu\) as a diagnostic function of \((M_i/M_j)^{(k-j)}\). Sets of curves for these values, corresponding to the profiles in Fig. 13, are plotted in Fig. 14. While there is clearly a relationship between the two quantities, the spread in the curves and the changes in time imply that a trial-and-error approach is ultimately required to determine a specific functional relationship. The curves were used as guidance, with the ultimate criterion being the closeness of the results to the reference solution, to determine the following proposed parameterization:

\[
\mu = 11.8 \left[ 100 \left( \frac{M_k}{M_j} \right)^{(k-j)} - 0.7 \right]^2 + 2. \tag{10}
\]

This diagnostic equation is applied to the scheme at the beginning of each time step. The function is denoted by the heavy curve in Fig. 14. For comparison, the diagnostic relationships for \(\mu = f(M_0, M_3)\) from MY05a and from Seifert (2008, hereafter S08), which were determined in a similar fashion (but based on \(D_m\)), are also plotted. The proposed relationship better captures the narrow distributions (large values of \(\mu\)) associated with very small values of \((M_i/M_j)^{(k-j)}\) compared to MY05a. While the proposed parameterization also fits the data from our reference model better than the parameterization of S08, it must be recognized that S08’s diagnostic relation was based on results from a spectral model simulation for rain that included, in addition to sedimentation, the processes of drop coalescence, collisional breakup, and evaporation. The parameterization of (10) does not account for these other processes that affect the narrowness of the PSD for rain. However, the approach to deriving (10) is applicable in general for the sedimentation of any hydrometeor category.

The error plots for various two-moment simulations, including the integrations using the diagnostic-\(\mu\) approaches, are shown in Fig. 15. Errors in the higher-order moments are reduced by using larger constant values of \(\mu\) as shown for \(\mu = 0, 3, \text{ and } 6\) in Figs. 15a–c. The runs with the diagnostic relations of MY05a and S08, shown in Figs. 15d and 15e, respectively, differ from the fixed-\(\mu\) runs (Figs. 15a–c) in that they do not overpredict the high moments, owing to the higher allowable values of \(\mu\) (Fig. 14), though there is an underprediction below the leading edge of the profile. The \(M_0-M_3\) run using the diagnostic relation (10) is shown in Fig. 14f. Overall, there is less error with the proposed parameterization than with the fixed-\(\mu\) runs or with the other diagnostic-\(\mu\) approaches (Table 1). Based on the error metric, this run ranks much better than the two-moment fixed-\(\mu\) integration and is even better then several of the three-moment runs presented.

To illustrate the generality of the new parameterization, the error plots for the \(M_0-M_2\) run using (10) are
shown in Fig. 14g. This configuration is chosen since the $M_0-M_2$, $\mu = 0$ run had the worst error score (Table 1). Clearly, the new parameterization is better than the fixed-$\mu$ approach and is an improvement over the diagnostic-$\mu$ equation proposed by MY05a (Fig. 14; Table 1). It also has the advantage of being general for a two-moment scheme with any choice of prognostic moments, where the choice of moments other than $M_0$ and $M_3$ may lead to errors in $D_m$, which is computed directly from $M_0$ and $M_3$ from (3), on which MY05a’s diagnostic equation depends.

Despite its simplicity, the proposed diagnostic-$\mu$ parameterization works well for this simple idealized case, and indeed the application of the MY05a relation allowed a two-moment scheme to produce similar results to the three-moment version in a full-physics 3D simulation of a hailstorm (Milbrandt and Yau 2006a,b). Nevertheless, it should be recognized that other microphysical processes besides sedimentation act to alter the PSD (for all hydrometeors). Ultimately, a diagnostic-$\mu$ parameterization should be determined from output of full-physics three-moment simulations, where the evolution of $\mu$ from all important processes is properly modeled, or from a detailed bin-resolving model, following the approach of S08.

c. Alternative approach for a fixed-$\mu$ scheme

While the diagnostic-$\mu$ approach is an improvement over the standard two-moment method for modeling sedimentation, there may be reasons against using a variable $\mu$. For example, a BMS may be hard-coded to have a constant value of $\mu$, either for considerations of code optimization or because a scheme’s original design assumed inverse-exponential PSDs. Furthermore, observations support a more restrictive spectral dispersion for some hydrometeor categories, such as snow (e.g., Heymsfield et al. 2008), so too much variability in $\mu$ may
be deemed physically unrealistic. For such two-moment schemes, it is still possible to control the problem of excessive size sorting while maintaining a fixed value of $\mu$.

The following approach to modifying the standard computation of sedimentation can be applied for any two-moment $M_j$-$M_k$ scheme, where $j < k$. First, $V_k$ is computed as normal from (8) using the prescribed value of $\mu$ assumed in the BMS. A value of $\mu'$ is then computed from (10), which is then used in place of $\mu$, along with the computed value of $V_k$, to compute $V_j$ from (9). The fall velocity for the higher moment is thereby computed based on the standard method, but the fall velocity for the lower moment approaches that of the higher moment as $D_m$ increases, thus reducing differential sedimentation and the rate of size sorting. For example, for a standard $M_1$-$M_3$ scheme with a fixed $\mu = 0$, where $D_m = 0.0013$ m, $V_3$ is the mass-weighted bulk fall speed for $M_3$ (computed using $\mu = 0$), $\mu' = 6$ (Fig. 14), and the computation of $V_0$ would be computed such that $V_3/V_0 = 1.2$ (Fig. 12), implying a slower rate of size sorting than if $V_3/V_0 = 2.2$, as it would with the standard calculation, using $\mu = 0$.

This approach—despite some inconsistency between the value of $\mu$ used in the computation of the ratio of the bulk fall velocities and that used in the rest of the scheme—has the redeeming quality that it is very effective in mitigating the problems associated with excessive size sorting in a standard fixed-\(\mu\) two-moment scheme and in reducing the errors in most of the computed moments (Fig. 15h) compared to the standard approach (Figs. 15a–c). According to Table 1, this approach in fact demonstrates this approach is very effective in reducing errors in the moments from (9). The following approach to modifying the standard computation of sedimentation can be applied for any two-moment $M_j$-$M_k$ scheme, where $j < k$. First, $V_k$ is computed as normal from (8) using the prescribed value of $\mu$ assumed in the BMS. A value of $\mu'$ is then computed from (10), which is then used in place of $\mu$, along with the computed value of $V_k$, to compute $V_j$ from (9). The fall velocity for the higher moment is thereby computed based on the standard method, but the fall velocity for the lower moment approaches that of the higher moment as $D_m$ increases, thus reducing differential sedimentation and the rate of size sorting. For example, for a standard $M_1$-$M_3$ scheme with a fixed $\mu = 0$, where $D_m = 0.0013$ m, $V_3$ is the mass-weighted bulk fall speed for $M_3$ (computed using $\mu = 0$), $\mu' = 6$ (Fig. 14), and the computation of $V_0$ would be computed such that $V_3/V_0 = 1.2$ (Fig. 12), implying a slower rate of size sorting than if $V_3/V_0 = 2.2$, as it would with the standard calculation, using $\mu = 0$.

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Note that the above test was performed with the tacit assumption that it is the low value of the lower moment’s bulk fall velocity $V_j$ that is problematic, not $V_k$. In fact, since the excessive size sorting comes from too large a value of the ratio $V_k/V_j$, the mitigation approach could just as easily be achieved by reducing $V_k$, or by both increasing $V_j$ and reducing $V_k$ appropriately, provided that the ratio decreases.

5. Conclusions

The effects of the choice of prognostic moments in one-, two-, and three-moment bulk schemes for the simulation of pure sedimentation were examined in the context of a simple column model, where all other microphysical processes were inactive. Using a reference solution from an analytic spectral model, the relative errors in the moments from $M_0$ to $M_7$ from the bulk scheme simulations were computed. While all of the calculations were done for rain, the conclusions apply equally to all sedimenting hydrometeor categories. Despite several advantages of two-moment schemes over the one-moment schemes (e.g., see MY05a for discussion), the standard two-moment bulk approach—with the total number concentration $M_0$ and the mass mixing ratio $M_3$ predicted and the relative spectral dispersion $\mu$ held constant—produces considerable error in the computed (nonprognostic) moments, with underprediction in the moments on which the microphysical growth rates depend ($M_1$–$M_2.5$) and severe overprediction of the higher-order moments, including reflectivity $M_6$. This is largely due to uncontrolled size sorting and the inability of a fixed-$\mu$ scheme to reproduce the narrowing of the particle size spectrum with time. A three-moment scheme is dramatically better than a one- or two-moment scheme at correctly simulating the entire range of moments considered, with the $M_1$–$M_5$–$M_7$ prognostic moment combination having the least amount of error for the configurations tested in this study, according to the error metric used.

Despite the demonstrated advantages of predicting all three free parameters of the PSD, the use of a full three-moment BMS in a 3D atmospheric model is considerably more expensive computationally than a two-moment scheme with the same number of hydrometeor categories because of the additional variables that must be advected by the model dynamics. Furthermore, it would require a considerable amount of code modification to an existing two-moment scheme to add all of the microphysical equations for a third set of prognostic moments. Two techniques for controlling size sorting in a two-moment BMS have been proposed and evaluated, one using a diagnostic shape parameter and the other reducing the differential fall velocities. The diagnostic-$\mu$ parameterization proposed in this study could be easily added to most existing two-moment BMSs. As demonstrated, this approach is very effective in reducing errors that result from excessive size sorting. For a two-moment scheme that must contend with a constant $\mu$, such as those hard-coded for inverse-exponential PSDs, the proposed approach for using a diagnostic $V_j/V_i$ ratio is an effective alternative for improving the computation of sedimentation of rain in a two-moment scheme and is very simple to implement.

We note in passing that sedimentation in a one-moment BMS could also possibly be improved by varying the size distribution parameters. Fixing $n_0$ as a constant is not an intrinsic requirement of a one-moment scheme and indeed this is not always done (e.g., Thompson et al. 2004). However, given that any one-moment scheme has, by definition, only 1 degree of freedom, it seems unlikely
that the computation of sedimentation can be significantly improved. Attempts to explore this are beyond the scope of this study.

For the scheme configurations tested, the overall skill in terms of predicting a large range of moments has been ranked. Some limitations of this framework must be recognized. First, although a broad selection of prognostic moment values allowed us to examine the general behavior of the solutions, only a subset of the infinite number of possible moment combinations were tested. Second, the importance of errors in some computed moments will vary depending on the application of the model. For example, errors in the higher moments such as \( M_6 \) (reflectivity) are an important consideration if radar reflectivity is assimilated in the model or if model equivalent reflectivity is a valued diagnostic field, but they may otherwise be deemed to be acceptable since they do not contribute to prediction errors in fields such as precipitation rates. Thus, model developers should take the ultimate goals of the modeling system into account when considering designing or modifying a BMS, in terms of the choice of prognostic moments.

The results presented in this study and in that of WL09 regarding the choice of prognostic moments for microphysics parameterizations do not apply only to the development of a new scheme. An existing BMS, such as a two-moment \( M_0-M_3 \) scheme, could be readily modified to use other moments as the prognostic variables (i.e., the quantities that get advected by the dynamical model) without actually having to change the microphysical source and sink terms, which are already formulated for \( M_0 \) and \( M_3 \). Upon entering the microphysical growth rate section of the BMS, the DSD parameters would be computed from the (new) prognostic moments. These would be used to compute \( M_0 \) and \( M_3 \) and subsequently the changes to \( M_0 \) and \( M_3 \) due to microphysical growth. The changes to the prognostic moments can then easily be calculated, followed by sedimentation of those moments. Alternatively, a two-moment \( M_0-M_3 \) scheme could be modified to use the pair of moments best suited for sedimentation to compute sedimentation only. Conservation of \( M_3 \) in each column could then be imposed if global conservation of mass is deemed necessary.

Examination of these approaches to testing alternative prognostic moments in full-physics simulations with a two-moment \( M_0-M_3 \) BMS and a three-moment \( M_0-M_3-M_6 \) BMS will be the topic of a future study.

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APPENDIX A

Computation of the Reference Solution

The spectral model results are obtained as follows. The PSD is discretized into 5000 size bins with diameters ranging from 0 to 10 mm (and thus a bin width of 0.002 mm). From the initial size distribution, given by (1), the number concentration \( N_i(D_i) \) in each bin \( i \) at each level is known. The empirical velocity–diameter relation for the sedimentation velocity of rain \( V \) takes the form of the power-law relation

\[
V(D) = \gamma a D^b,
\]

where \( a = 130 \, \text{m}^{0.5} \, \text{s}^{-1} \), \( b = 0.5 \) (Kessler 1969), and \( \gamma = (\rho / \rho_0)^{0.5} \) is the air density correction factor (with \( \rho \) and \( \rho_0 \) denoting the air density aloft and at the surface, respectively) which, for simplicity, is assumed to be 1 throughout this study, as in MY05a and WL09.

For a given future time, the height to which the particles in each bin fall is computed from

\[
z_i(t) = z_{i0} - V_i(D_i) t, \tag{A2}
\]

where \( z_i(t) \) is the height to which the particles in bin \( i \) fall after time \( t \), \( z_{i0} \) is their initial height, and \( V_i(D_i) \) is the sedimentation velocity of the drops, with \( D_i \) the diameter for the drops in the bin, given by (1). At time \( t \), the \( k \)th moment \( M_k \) is computed from

\[
M_k(z,t) = \sum_i D_i^k N_i(D_i,z,t) \Delta D. \tag{A3}
\]

The solution for the spectral model at any time \( t \) is obtained analytically using (A1) and (A2); no time-stepping is performed. This is straightforward since \( V_i(D_i) \) does not change in time or space because of the lack of interaction between particles and the assumption of a constant air density. A simple summation using (A3) is used to determine profiles of any moment \( k \).

APPENDIX B

Computation of the Size Distribution Function Parameters

For the gamma function given by (1), the size distribution parameters are solved based on the values of the prognostic moments and the appropriate closure assumptions as follows.

For a one-moment scheme, with prognostic moment \( M_1 \), the closure assumptions \( \mu = 0 \) and \( n_0 = 8 \times 10^6 \, \text{m}^{-4} \) (see main text) are made and \( \lambda \) is then solved by
\[ \lambda = \left[ n_0 \frac{\Gamma(j + \mu + 1)}{M_j} \right]^{(j+\mu+1)}. \] (B1)

For a two-moment scheme, with prognostic moments \( M_j \) and \( M_k \), \( \mu \) is first prescribed by the chosen closure assumption, either as a prescribed constant or as a diagnostic function of \( M_j \) and \( M_k \) (as discussed in section 4). The remaining size distribution parameters are then computed from

\[ n_0 = \frac{M_j}{\Gamma(j + \mu + 1)} \gamma^{(k+\mu+1)/(k-j)} \times \frac{M_k}{\Gamma(k + \mu + 1)} \gamma^{-(j+\mu+1)/(k-j)}. \] (B2)

and from (B1).

For a three-moment scheme, with prognostic moments \( M_j, M_k, \) and \( M_l \), \( \mu \) is first computed by solving, through iteration,

\[ M_j^{(l-k)/(k-j)} M_k^{(j-l)/(j-k)} M_l = \Gamma(j + \mu + 1)^{(l-k)/(k-j)} \times \Gamma(k + \mu + 1)^{(j-l)/(j-k)} \times \Gamma(l + \mu + 1), \] (B3)

which is derived from (4), (B1), and (B2); \( \lambda \) and \( n_0 \) are then computed by (B2) and (B1), respectively.

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