Development of NTU triple-moment ice-phase microphysics scheme with consideration of particle shape and density variation

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Abstract

A physics-base cloud microphysical parameterization was developed by the National Taiwan University (NTU) and implemented into the WRF model. This NTU scheme considers two classes of liquid-phase hydrometeors (cloud drop and raindrop) using double-moment representation, and 4 classes of ice-phase hydrometeors (pristine cloud ice, snow aggregate, rimed ice, and hail) using triple-moment representation. Furthermore, shape (aspect ratio) and density variations are considered for cloud ice and snow aggregate; while rimed ice (graupel) also considers density changes. The liquid-phase parameterization was derived from binned microphysics models, while the ice-phase scheme follows traditional bulk parameterization but with improved representation of size spectrum and physical mechanisms, the latter include full interaction with condensation nuclei and ice nuclei. Our scheme has been applied in several cloud systems, all showing satisfactory results especially in the radar reflectivity analysis.

1. Introduction

To simulate accurately cloud and precipitation formation, cloud models need to consider not only various physical mechanisms but also the heterogeneity of the cloud particles, such as the differences in phase, size and chemical contents. These particle properties are so diverse and yet play critical roles in essentially all microphysical processes. However, an ordinary-sized convective cumulus easily contains over 10^{20} particles, which are very difficult to track individually in numerical models. Therefore, cloud microphysical models need to simplify the system by grouping the particles into manageable number of categories. The first level of grouping is to differentiate particles according to the phase of hydrometeors, primarily ice phase or liquid phase, and can be refined if necessary (e.g., into cloud drops and raindrops for the liquid-phase, and into cloud ice, snow, graupel and hail for the ice phase). The second level of grouping is to categorized particles in each hydrometeor types according to their sizes, the combination of which composes the so-called size distribution. More sophisticated cloud models applied the “bin method” to describe the size distribution in a size (or mass) coordinate (e.g., Clark, 1973; Hall, 1980; Khain et al., 1996, 2004; Lynn et al., 2005). Particles are grouped into a certain bin if their sizes (or masses) lie within this bin’s size range. Typically, tens to over 100 size categories (note: Khain et al. 2015 suggested > 40), depending on the numerical method that applied for the mass advection, are needed to describe the size distribution properly. So, although the bin models are considered more accurate, their high computational burden prevented application for operational weather forecasting.

Another kind of approach, first proposed by Kessler (1969), is the so-called “bulk parameterization” which utilized relatively simple mathematical functions to describe the size distribution (see Fig. 1 for the contrast between bin method and bulk method). Each mathematical function can be described with less than a handful of variables (mostly 1 or 2). Furthermore, cloud particles tend to have multiple populations (modes) in terms of size, therefore, the bulk approach requires more than one hydrometeor types to describe the particle spectrum. For example, the bulk model must use separate categories of “cloud drop” and “raindrop” to describe the full size distribution of liquid-phase drops, whereas the bin models apply continuous bin categories to cover all water drops. Earlier bulk parameterization tracks only a single properties (called the “moments”) of each hydrometeor categories. This limited their capability to simulate the evolution of cloud particle size spectra. Now, more and more cloud microphysical schemes shifted to the double-moment method. This study presents the development of a new multi-moment microphysics scheme developed in-house by the Cloud and Aerosol Research Laboratory at the National Taiwan University.

The first version of the NTU scheme (NTU-v1) contains a two-moment bulk warm cloud scheme, which explicitly predicting the mass and the drop number of cloud drops and raindrops. The warm cloud scheme is based on the scheme of Chen and Liu (2004) (hereafter called the CL scheme) which applied a multi-component bin microphysical model and then statistically fit the simulation results into bulk formulas. So, the CL scheme neither assumes a specific size distribution for cloud drops and raindrops nor simplifies the growth kernel as done in traditional bulk parameterization. For CCN activation, the minimum size of dry aerosol to be activated depends on supersaturation according to the Köhler equation. An embedded Lagrangian ascending air parcel is applied to better resolve the supersaturation and thus the activation process. The remaining microphysical processes are calculated in an Eulerian framework after CCN activation and diffusional growth of hydrometeors are accounted for. The CL scheme also allows the activation of giant CCN into rain embryos which, in additional to the autoconversion, is an important warm rain initiation process. The CL scheme keeps track of solute in cloud drops and raindrops such that restoration of aerosol from drop evaporation is allowed. In NTU-v1, the CL scheme is coupled with the mixed-phase cloud parameterization of Reisner et al. (1998) with some modifications (Cheng et al. 2010). Ice-phase hydrometeors that considered including the number and mass concentrations of cloud ice, snow and graupel/hail. The ice nucleation processes are modified according to the methods of Chen et al. (2008) with which the effect of various types of ice nuclei can be calculated according to the stochastic nucleation theory. Other modifications to the Resner et al. (1998) scheme include the homogeneous nucleation and rain production from snow melting (see Cheng et al. 2010 for details).

In the second version of NTU scheme (called NTU-v2), the CL scheme is retained because of the robust performance, but the Reisner et al. (1998) mixed-phase parameterization is replace with that developed by Tsai (2014). The replacement was done to reduce model uncertainties and errors, particularly those related to mathematical and physical representations. Furthermore, the NTU-v2 scheme is one of the first bulk parameterization to consider the ice crystal growth habit (shape) effects by adopting the parameterization method of Chen and Tsai (2016). Also, a new hydrometeor category -- hail – was added to improve the simulation precipitation formation in severe convections.

2. Method

The development of bulk parameterization was based on a couple of key assumptions: 1) the shape of the prescribed size distribution function (e.g., the Marshall-Palmer distribution) can be maintained throughout the cloud lifetime, and 2) the rate of conversion between hydrometeors (including water vapor) can be derived either theoretically or empirically. For example, the most commonly used size spectrum is the Marshall-Palmer distribution,

$$n(r) = N_0 \exp(-\lambda r) \tag{1}$$

where $n(r)$ is the number density function, r is the radius, N_0 and λ are variables commonly called the intercept and slope, as $n(r)$ is a straight line when expressed in logarithmic scale. The "bulk" properties of any particular hydrometeor type can be expressed in terms of the "moment" of the distribution; that is, the k^{th} moment is written as:

$$M_k = \int_0^\infty r^k n(r) dr \qquad (1)$$

Specifically, the concentration of total number, surface area, volume and radar reflectivity factor are represented by the 0^{th}, 2^{nd}, 3^{rd} and 6^{th} moments, respectively.

Assumption 1) limited the degree of freedom for the evolution of size distribution. For example, the Marshall-Palmer distribution mentioned above is empirically determined from observed raindrop size spectrum but is often inappropriately applied to other hydrometeors. Furthermore, earlier bulk parameterization considered only the total mass (and thus volume if the density is fixed) of the hydrometeors, so there is only one known parameter to solve Eq. (2) from Eq. (1) which contains two variables. Therefore these schemes must keep one variable constant (usually N_0, as done in the Kessler's scheme) or somehow diagnose N_0 from other variables. This would results in large errors as many studies show that N_0 does vary significantly. To better resolve the evolution of size distribution, more advanced bulk parameterization scheme track an additional bulk property, usually the total number concentration (0^{th} moment), with which both N_0 and λ can be solved. This would also enable the interaction between aerosol and cloud. Yet, more advanced (than Marshall and Palmer's era) raindrop size spectrum measurements indicated that Eq. (1) tends to exaggerate the number of small raindrops. A better representation is the gamma-type function that applied in the NTU-v2 scheme:

$$n(r) = N_0 r^\alpha \exp(-\lambda r) \tag{3}$$

where α is called the shape (spectral width) parameter. Parameters N_0, λ and α can be derived from three known moments using solutions provided in Chen and Tsai (2016).

Conventional bulkwater schemes usually assumed constant density for each hydrometeor. However, density of ice hydrometeors tends to vary significantly during growth, and many microphysical parameters (such as fall speed, optical properties, radar reflectivity) are rather sensitive to particle density. To resolve density variation, the NTU-v2 scheme tracks the total volume, with which density can be diagnosed with the mass information. Note that the third moment of size distribution is directly proportional to volume instead of mass.

Another special feature of the NTU-v2 scheme is the different definition of several ice-phase hydrometeors. The "cloud ice" category commonly used in bulkwater schemes is redefined as "pristine cloud ice" which grows only by vapor diffusion; the aggregation of pristine cloud yields snow aggregate, whereas riming produces rimed ice (which is also termed graupel here). Using this physical process-based definition, we eliminated the artificial process of autoconversioin between cloud ice and snow that is based on a specified size threshold; which means that, in our scheme, both cloud ice and snow have no upper and lower size limits). This also eliminated problem in mathematics associated with incomplete integration of size distribution (e.g., Marshall-Palmer) due to the artificial cutoff.

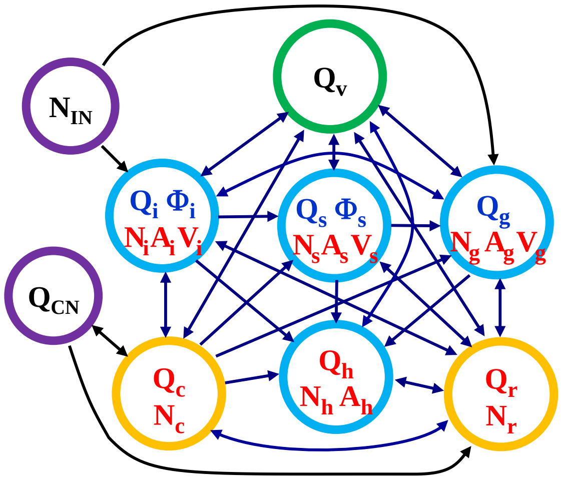

Figure 1: Schematic of the NTU bulk parameterization for cloud microphysics. Circles indicate hydrometeor/particle categories, including water vapor (v), cloud drop (c), raindrop (r), pristine cloud ice (i), snow aggregate (s), rimed ice/graupel (g), hail (h), condensation nuclei (CN) and ice nuclei (IN). Symbols within the circles are major properties of hydrometeors, with N, A, V, Q, Φ for total number, area, volume, mass (mixing ratio), and shape (volume-weighted aspect ratio), respectively. Among them, N, A and V are the three moments that used for describing the size distribution. For cloud drop, raindrop and hail, volume is diagnosed from mass by assuming fixed density.

Table 1: Summary of the classification and properties of hydrometeors in the NTU-v2 scheme.

	cloud drop	rain	cloud ice	snow	graupel	hail
definition	D<100 mm	D≥100 mm	pristine ice crystal	Ice crystal aggregates	rimed ice	$D > D_{SLL}$
moment	2	2	3	3	3	3
Shape	spherical	spherical	variable	variable	spherical	spherical
density	1000 kg/m^3	1000 kg/m^3	variable	variable	variable	900 kg/m^3

*D_{SSL}: Shumann-Ludlam size limit

The second basic assumption is the availability of analytical solution to the conversion rate (for each moment). In fact, the most difficult and elaborate task in developing bulk microphysics scheme is to determine the rate change of moments ($\frac{dM_k}{dt}$) due to various physical processes. For single-body (non-collision type) processes, the conversion rate can be expressed as:

$$\frac{dM_k}{dt} = \int K_k \, n(r)dr = \int \frac{dr^k}{dt} \, n(r)dr \tag{4}$$

where K_k is the "kernel" of growth (meaning the rate change of particles of a certain size r). For example, the kernel for vapor diffusion (condensation) growth is expressed as (cf. Pruppacher and Klett, 1997):

$$\frac{dm}{dt} = 4\pi r D f_g f_v (\rho_{v,\infty} - \rho_{v,p}) \tag{5}$$

where D is the diffusion coefficient, f_g is the modification due to the gas kinetic effect (Fuchs, 1959; Fuchs, 1964), f_v is the ventilation coefficient, which can be ignored for small aerosol particles; $\rho_{v,\infty}$ is the ambient vapor density, and $\rho_{v,p}$ is the surface vapor density. The terms f_g, f_v and $\rho_{v,p}$ are size dependent, such that the growth kernel is rather nonlinear with respect to r. For collisional processes, the rate change of moments involves double integrals over the size spectra of the two involving hydrometeor modes (e.g., mode A and mode B). For coagulation between two particles of sizes r_A and r_B, the coagulated particle has a size $r_C = (r_A^3 + r_B^3)^{1/3}$. It follows that the changes in their k^{th} moments are $-r_A^k$ and $-r_B^k$, respectively, for each original particle, and $+r_C^k$ for the coagulated particle. Then, the fundamental equation for coagulation between particles in the collector mode *A* and the contributor mode *B* can be expressed as

$$\frac{dM_{k,A}}{dt} = \iint \left[r_C^k - r_A^k \right] K(r_A, r_B, C_{air}) n_A(r_A) n_B(r_B)\, dr_A dr_B \tag{6}$$

$$\frac{dM_{k,B}}{dt} = \iint \left[-r_B^k \right] K(r_A, r_B, C_{air}) n_A(r_A) n_B(r_B)\, dr_A dr_B \tag{7}$$

Here, the collision kernel $K(r_A, r_B, C_{air})$ has complicate dependences on the colliding particle sizes (r_A and r_B) as well as air temperature and pressure (denoted as C_{air}). Due to the high nonlinearity of such kernels, exact analytical solutions for Eqs. (5)-(7) are not available. For the bulk scheme to work, these kernels must be simplified, and this is a main source of error for the bulk parameterization. Details of the simplifications commonly used in current bulk schemes will not be elaborated here. Instead, here we focus on methods for possible improvements.

Chen et al. (2013) proposed a few methods to transform the complicated conversion rates into more manageable forms but maintain high accuracy. Although the methods were developed for aerosol microphysics, they are equally suited for cloud microphysics. One of them is called the kernel transformation method, which transform the growth kernel into mathematical forms that allows analytical solution to Eqs. (5)-(7). Chen and Tsai (2016) successfully adopted this method to convert the highly complicated electrostatic capacitance factor for the vapor diffusion growth of non-spherical ice particles. The other methods (called integral transformation and optimal-size approximation) applied statistical analysis on the numerical solutions of the conversion rates and then apply multi-variable fitting to yield more efficient formulas for the conversion rates. This study adopted these methods for improving the mixed-phase collision processes whose kernels are highly simplified in current bulk schemes.

The NTU-v2 scheme further enhanced the ice-phase hydrometeor mechanisms. Here we briefly describe the improvements that are of special interest to this study.

a. Ice nucleation

Heterogeneous ice nucleation process is responsible for ice particle initiation in clouds warmer than -40℃. This process requires the presence of ice nuclei (IN). Klein et al. (2009) and de Boer et al. (2010) pointed out that, because of insufficient knowledge about IN, mixed-phase processes are often difficult to simulate. In fact, current weather forecasting models generally do not explicitly consider IN. Most of them applied empirical formulas that derived from field measurements, which often show large variabilities. Yet, the microphysical scheme commonly applied a fixed formula which lacks of general applicability in space and time (Tao et al., 2012). The NTU-v2 scheme incorporated the generalized parameterization of Chen et al. (2008), which keeps the original mathematical form of the classical nucleation theory and includes thermodynamic parameters of the IN (i.e., contact angle and activation energy) derived from laboratory measurements for various types of IN, such as mineral dust, soot, bacteria, pollen, etc. In this way, the calculation of ice nucleation can be based on simulated IN or best estimates of IN species and concentrations.

In Chen et al. (2008), the heterogeneous ice nucleation rate is generalized into the following form:

$$J_{HN} = 4\pi r_{IN}^2 A \sqrt{f} \exp\left(\frac{-\Delta g_a - f \cdot \Delta g_g}{k_B T} \right) \tag{8}$$

where r_{IN} is the radius of the ice nuclei, *A* is a parameter that depends on the ambient conditions only, *f* is a size-dependent geometric factor, Δg_a is the activation energy, Δg_g is the homogeneous germ formation energy, and k_B is the Boltzmann constant. The IN-specific thermodynamic parameters are contained in factors *f* and $-\Delta g_a$, the values of which have been provide by Chen et al. (2008) and Hoose et al. (2010) for many IN species. The overall nucleation rate for a population of ice nuclei is then expressed as

$$I_k = \int J_{HN} \cdot r_{IN}^k \cdot n(r_{IN}) dr_{IN} \tag{9}$$

where $n(r_{IN})$ is the size distribution of the ice nuclei. Note that one of the NTU version of WRF already included the dust emission and dust-cloud interaction mechanisms (Lin, 2015), and thus is suitable for evaluation the role of IN this study. Mechanisms for other IN species are currently developed and to be built into this NTU version of WRF.

b. Ice crystal shape

All other conditions being equal, the shapes of ice crystals can lead to considerable differences in the vapor diffusional growth of ice crystals, their terminal velocity, the collision efficiency, and the optical properties (cf. Chen et al., 2016). Yet, most of the current cloud models assumed that cloud ice particles are spherical (e.g., Lin et al., 1983). The few that did considered the possibly eccentricity of ice crystal shapes tended to ignore the “memory” of crystal shape, meaning that their growth history and the time required for shape adjustment are not considered. Harrington et al. (2013) and Chen et al. (2016) showed that ignoring the shape effect would result in large error in the growth of cloud ice crystal. As most of the large ice particles (i.e., snow, graupel and hail) were initiated from cloud ice, the inaccuracy associated with the spherical ice assumption tends to propagate to precipitation formation. So, the NTU-v2 scheme applied the ice shape parameterization method that developed by Chen and Tsai (2016).

The basic shape of an ice crystal (commonly referred to as the primary growth habit) can be characterized with the aspect ratio:

$$\phi \equiv c / a \tag{10}$$

where *c* is the semi-dimension of the axis perpendicular to the basal face, and *a* is the semi-dimension of the axis perpendicular to the prism-face (length from the center to the corner). Chen and Lamb (1994) derived the relationship that describes the relative changes in the axes lengths:

$$\frac{d\ln c}{d\ln a} = \gamma \tag{11}$$

where γ is the ratio of the accommodation coefficient at the basal face to that at the prism face. This "inherent growth habit" is driven by surface kinetic processes and is primarily a function of temperature. Chen and Tsai (2016) applied an "associated property" referred to as the "shape moment", which is defined as a volume-weighted aspect ratio:

$$M_{\phi} \equiv \int \phi D^3 n(D) dD = D_0^{-3\zeta} M_{3\zeta+3}. \tag{12}$$

With this shape moment, the changes in moments due to vapor deposition (for which the 0^{th} moment remain constant) can be expressed as (cf. Chen and Tsai, 2016):

$$\frac{dM_2}{dt} \equiv \int \frac{dD^2}{dt} n(D) dD = \int \frac{2}{3D} \frac{dD^3}{dt} n(D) dD = \frac{16 D_v' \Delta\rho_v}{\rho_{dep}} \int \frac{C_E f_v}{D} n(D) dD \tag{13}$$

$$\frac{dM_3}{dt} \equiv \int \frac{dD^3}{dt} n(D) dD = \frac{6}{\pi \rho_{dep}} \int \frac{dm}{dt} n(D) dD = \frac{24 D_v' \Delta\rho_v}{\rho_{dep}} \int C_E f_v n(D) dD \tag{14}$$

$$\frac{dM_{\phi}}{dt} = \int \frac{d(\phi D^3)}{dt} n(D) dD = \int \frac{d\phi}{dt} D^3 n(D) dD + \int \phi \frac{dD^3}{dt} n(D) dD \tag{15}$$

Semi-analytical solutions for the above equations have been derive by Chen and Tsai (2016) and thus will not be elaborated here. Chen and Tsai (2016) showed that, by including the shape moment, the error in mass growth reduces from 45% to less than 1%.

3. Model performance

Here we use the MC3E (the Midlatitude Continental Convective Clouds Experiment) case for demonstration of the NTU scheme's performance. This case occurred in the southern Great Plain in 2011, and is viewed as a "Dream Scenario" for cloud model evaluations. Figure 2 presents the precipitation rate during the day, showing that the model roughly captured the major peak in the afternoon particularly for the simulation using more polluted aerosol initial condition. The clean aerosol condition tends to produce much too strong first peak.

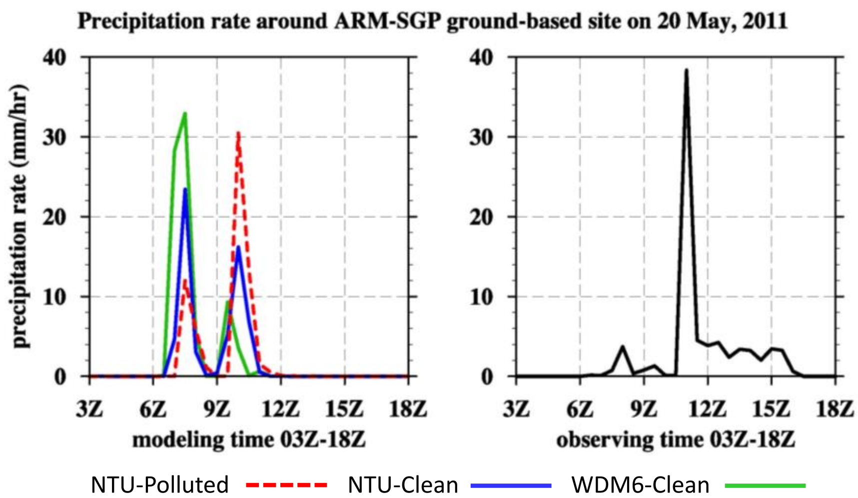

Figure 2: Left: hourly precipitation rates for the MC3E case simulated using the WDM6 scheme with clean aerosol (green), using NTU scheme with clean and polluted aerosols (blue and red, respectively). Right: observed precipitation rate.

The contoured frequency by altitude diagram (CFAD) of radar reflectivity in Fig. 3 shows that the NTU scheme produced better vertical profiles (correlations > 0.75) than the WDM6 scheme (correlation 0.49), with steeper vertical slope of high frequencies zone and closer to the observation. Obviously, microphysical parameterization has strong impact on not only surface precipitation amount but also the cloud vertical structure.

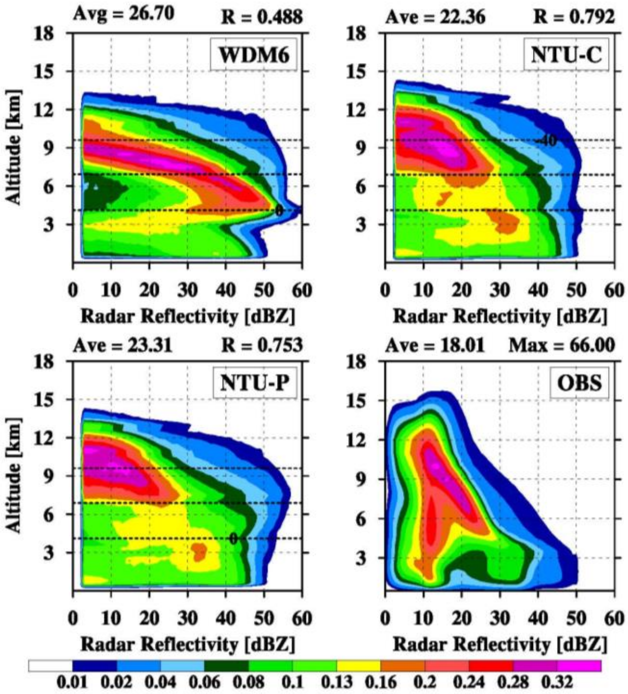

Figure 3: Contoured frequency by altitude diagram (CFAD) of radar reflectivity for the MC3E case using the WDM6 scheme and NTU scheme with clean-type aerosol (NTU-C) and polluted-type aerosol (NTU-P). Observation is shown in the lower right panel.

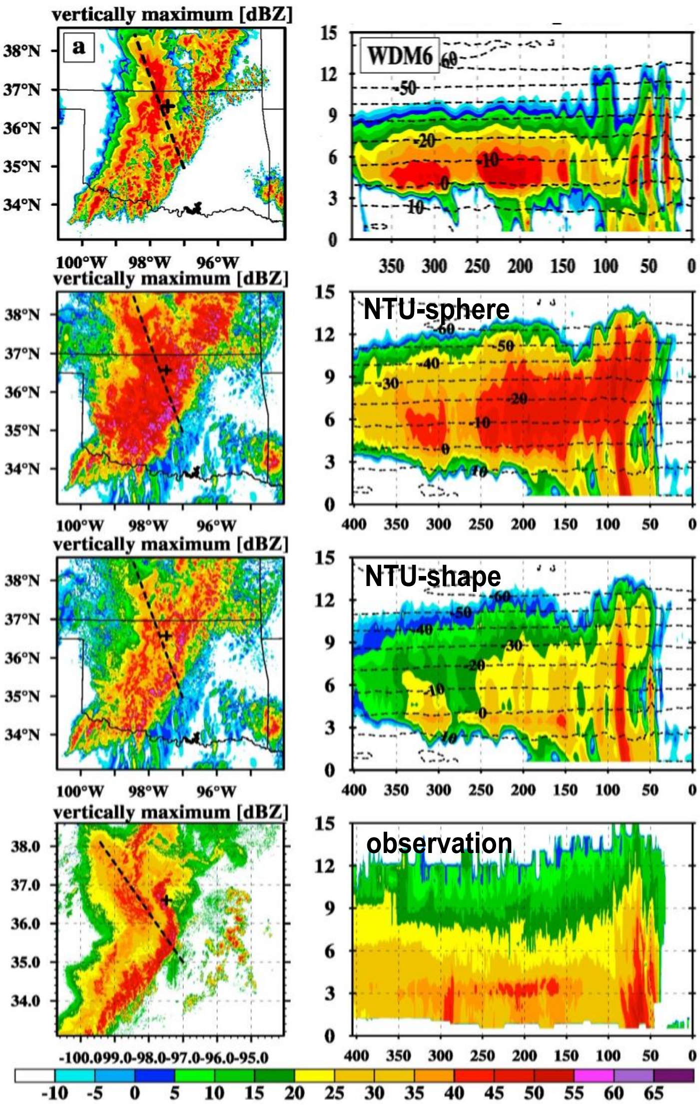

Figure 4: Projected maximum radar reflectivity (left) and vertical scan (right) from WDM6 run (top panel), NTU-C run (middle two panels) and observation (bottom). Radar reflectivity from NTU scheme was calculated by assuming all hydrometeors are spherical (2nd row) or with shape consideration (3rd row).

Another possible source of discrepancies between simulation and observation is the assumption of spherical particle shape in microphysical schemes. The scattering amplitude of radar signal is very much dependent of the particle shape. Figure 4 demonstrates that the overestimation in radar reflectivity may be improved when the particle shapes are taken into consideration. Particle density is also important in calculating radar reflectivity, but the details will not be elaborate here.

4. Summary

The NTU-v2 scheme is developed for improving microphysical representation in the WRF model. This scheme used 5 particle properties, including 3 for describing the size distribution (i.e., triple-moment), for cloud ice, snow and graupel. The extra properties are used to allow representation of particle shape and density variations. The hail category is assumed to be spherical and with fixed density, whereas cloud drops and raindrops are described using two moments. Preliminary results indicate that the NTU scheme performed fairly well in simulating the MC3E case as well as other cloud systems (e.g., frontal clouds, squall lines, thermal convections, marine stratiform clouds, and snow storms; not shown). As computational cost is more than twice of other double-moment schemes, the NTU-v2 scheme is more suitable for research purposes than for weather forecasting.

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