Large-Eddy Simulations of Trade Wind Cumuli Using Particle-Based Microphysics with Monte Carlo Coalescence

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ABSTRACT

A series of simulations employing the superdroplet method (SDM) for representing aerosol, cloud, and rain microphysics in large-eddy simulations (LES) is discussed. The particle-based formulation treats all particles in the same way, subjecting them to condensational growth and evaporation, transport of the particles by the flow, gravitational settling, and collisional growth. SDM features a Monte Carlo–type numerical scheme for representing the collision and coalescence process. All processes combined cover representation of cloud condensation nuclei (CCN) activation, drizzle formation by autoconversion, accretion of cloud droplets, self-collection of raindrops, and precipitation, including aerosol wet deposition. The model setup used in the study is based on observations from the Rain in Cumulus over the Ocean (RICO) field project. Cloud and rain droplet size spectra obtained in the simulations are discussed in context of previously published analyses of aircraft observations carried out during RICO. The analysis covers height-resolved statistics of simulated cloud microphysical parameters such as droplet number concentration, effective radius, and parameters describing the width of the cloud droplet size spectrum. A reasonable agreement with measurements is found for several of the discussed parameters. The sensitivity of the results to the grid resolution of the LES, as well as to the sampling density of the probabilistic Monte Carlo–type model, is explored.

1. Introduction

This study presents a series of large-eddy simulations (LES) employing the particle-based and probabilistic approach for representing aerosol, cloud, and warm-rain microphysics introduced in Shima (2008) and Shima et al. (2009) and referred to as the superdroplet method (SDM). The simulations cover a 24-h-long evolution of a field of shallow convective clouds typical of the trade wind boundary layer.

The highlight of the paper is the discussion of the simulation results in context of several previously published analyses of in situ cloud measurements from the Rain in Cumulus over the Ocean (RICO) field study (Rauber et al. 2007). SDM features a continuous (as opposed to binned) representation of the particle sizes and diffusive-error-free numerical schemes for both condensational and collisional growth of particles. This results in the availability of high-spectral-resolution data on the shape of the particle-size distribution within a large range of particle sizes from unactivated aerosol through cloud droplets to drizzle and rain drops. In this paper the cloud and rain size spectra obtained in LES-coupled SDM simulations are analyzed with the aim of presenting quantities comparable to those measured during RICO using high-resolution optical cloud and precipitation size spectrometers such as the Fast Forward Scattering Spectrometer Probe (Fast-FSSP) and the two-dimensional stereo (2D-S) probe [see Brenguier et al. (1998) and Lawson et al. (2006), respectively]. Employment of SDM as opposed to bulk, multimoment, or bin microphysics makes it feasible to take into account in the comparison of a wider range of cloud microphysical parameters than in previous

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studies comparing LES results with RICO aircraft observations (Abel and Shipway 2007; van Zanten et al. 2011).

2. Methodology

a. The superdroplet method

SDM is a particle-based simulation technique in which each of the particles for which computations are made [superdroplets (SDs)] represents a multiplicity of real-world particles of the same size and same composition. Formulation of the method is given in Shima et al. (2009) and may be briefly outlined as follows. The framework of the method consists of two mutually coupled components: (i) an Eulerian fluid flow solver, and (ii) a Lagrangian particle-tracking logic-computing evolution of physical coordinates and physicochemical properties of a population of particles immersed in the flow. All particles are treated as spherical solution droplets (ammonium sulfate solution assumed herein). The coupling between the Eulerian and the Lagrangian components is bidirectional. The Lagrangian component feeds on the fluid velocity field in order to update the positions of the superdroplets and the thermodynamic fields to compute the condensational growth or evaporation rates. The Eulerian component feeds on the water vapor and heat source/sink rates resulting from condensation and evaporation of water on the particles. In the Lagrangian component, all SDs are subject to transport by the flow, gravitational settling, and condensational and collisional growth. The distinction between aerosol, cloud, drizzle, or rain particles is made only at the stage of model output analysis—not in the model formulation itself.

Such particle-based formulation belongs to a class of discrete parcel methods (Crowe et al. 2012). Analogous particle-based techniques were recently used in LES of precipitation-forming clouds by Andrejczuk et al. (2010) and Riechelmann et al. (2012); what distinguishes SDM, however, is the Monte Carlo–type representation of the particle-coalescence process (Shima et al. 2009, their sections 2.1.4, 4.1.4, and 5.1.3). A similarly formulated Monte Carlo scheme for particle collisions was recently used in context of LES of ice-phase clouds in Sölch and Kärcher (2010).

b. Model setup

The simulations are carried out using the Cloud-Resolving Storm Simulator [CReSS; Tsuboki (2008), his chapter 9.2 and references therein], which is a non-hydrostatic compressible-LES-type solver. Two types of moist processes representations are used: the SDM and a Kessler-type bulk scheme [Kessler (1995) and the references to the earlier works of the author therein] implemented following Klemp and Wilhelmson (1978, their section 2b). The simulations are carried out using the setup defined in van Zanten et al. (2011) and corresponding to the atmospheric state measured and modeled in context of the RICO field project (Rauber et al. 2007). The setup is designed as an idealized case based on the composite structure of the trade wind boundary layer following RICO observations discussed in Nuijens et al. (2009). In particular, there is no diurnal cycle and both the prescribed radiative cooling and the sea surface temperature are assumed to be constant. Throughout the simulations the heat and the moisture content in the model domain is sustained by using source terms mimicking large-scale advection. The setup defines, among other settings, initial piecewise linear profiles of potential temperature, specific humidity, wind characteristics, and large-scale forcings (van Zanten et al. 2011, their Fig. 2 and Table 2).

The only exceptions from the original setup is the domain size—a quarter of the original domain size was used (i.e., \(6.4 \times 6.4 \times 4 \text{ km}^3\) instead of \(12.8 \times 12.8 \times 4 \text{ km}^3\)). Tests with full domain size (not discussed herein) revealed that quartering the domain enlarges the fluctuations in time of cloud macroscopic properties; however, not to a level significant for the presented discussion. Three different settings of gridcell sizes were used: \(100 \times 100 \times 40, 50 \times 50 \times 20\), and \(25 \times 25 \times 10 \text{ m}^3\).

The total number of superdroplets used in a simulation is the number of grid cells in the domain times a constant referred to as the mean superdroplet number density per grid cell (SDND). Values of SDND vary from 8 to 512 in the simulations presented herein. The initial coordinates and sizes of particles are chosen randomly with uniform distribution in physical space and bimodal lognormal distribution in particle-size space [size spectrum as specified in van Zanten et al. (2011, their section 2.2.3)]. All particles are initially in equilibrium with ambient humidity. The probability of collisions and coalescence is defined following Hall (1980, his section 3d and references therein), hence no influence of turbulence on collisional growth is taken into account. A semi-Lagrangian advection scheme with cubic Lagrange interpolation and the Smagorinsky–Lilly first-order closure was used.

A list of model runs and their corresponding labels used throughout the paper is given in Table 1. The table lists different time steps used in the simulations—in SDM the time steps used for the Eulerian and the Lagrangian computations differ as the corresponding numerical stability constraints differ (Shima et al. 2009, their section 5).

3. Results: Cloud and precipitation macrostructure

Figure 1 presents time series of domainwide statistics of cloud cover (cc), liquid water path (LWP), and rainwater path (RWP). All quantities are labeled and
Table 1. List of model runs discussed in the paper. The run label denotes whether bulk (blk) or SDM (sdm) microphysics was used, as well as which grid resolution (coarse, middle, or high) and SDND (8, 32, 128, or 512) was chosen. Coarse resolution corresponds to a quarter of the domain from the original RICO setup (i.e., gridbox size of $100 \times 100 \times 40$ m$^3$ with $64 \times 64 \times 100$ grid points); the middle and high resolutions denote settings resulting in halved and quartered gridbox dimensions, respectively (with the domain size kept constant). For each simulation there are five time steps defined: long and short time step of the Eulerian component (the short one used for sound-wave terms), the time step used for integrating the condensational growth/evaporation equation, the time step used for solving collisional growth using the Monte Carlo scheme, and the time step for integration of particle motion equations. The last column lists mean superdroplet number densities per volume.

<table>
<thead>
<tr>
<th>Run label</th>
<th>Grid</th>
<th>$dx = dy$ (m)</th>
<th>$dz$ (m)</th>
<th>Time steps (s)</th>
<th>SD density (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>blk-coarse-8</td>
<td>$64 \times 64 \times 100$</td>
<td>100</td>
<td>40</td>
<td>1.00/0.100/1.0</td>
<td>—</td>
</tr>
<tr>
<td>sdm-coarse-8</td>
<td>$64 \times 64 \times 100$</td>
<td>100</td>
<td>40</td>
<td>1.00/0.100/0.25/1.0/1.0</td>
<td>$2.0 \times 10^{-11}$</td>
</tr>
<tr>
<td>sdm-coarse-32</td>
<td>$64 \times 64 \times 100$</td>
<td>100</td>
<td>40</td>
<td>1.00/0.100/0.25/1.0/1.0</td>
<td>$8.0 \times 10^{-11}$</td>
</tr>
<tr>
<td>sdm-coarse-128</td>
<td>$64 \times 64 \times 100$</td>
<td>100</td>
<td>40</td>
<td>1.00/0.100/0.25/1.0/1.0</td>
<td>$3.2 \times 10^{-10}$</td>
</tr>
<tr>
<td>sdm-coarse-512</td>
<td>$64 \times 64 \times 100$</td>
<td>100</td>
<td>40</td>
<td>1.00/0.100/0.25/1.0/1.0</td>
<td>$1.3 \times 10^{-9}$</td>
</tr>
<tr>
<td>sdm-middle-8</td>
<td>$128 \times 128 \times 200$</td>
<td>50</td>
<td>20</td>
<td>0.50/0.050/0.25/1.0/1.0</td>
<td>$1.6 \times 10^{-10}$</td>
</tr>
<tr>
<td>sdm-middle-32</td>
<td>$128 \times 128 \times 200$</td>
<td>50</td>
<td>20</td>
<td>0.50/0.050/0.25/1.0/1.0</td>
<td>$6.4 \times 10^{-10}$</td>
</tr>
<tr>
<td>sdm-middle-128</td>
<td>$128 \times 128 \times 200$</td>
<td>50</td>
<td>20</td>
<td>0.50/0.050/0.25/1.0/1.0</td>
<td>$2.6 \times 10^{-9}$</td>
</tr>
<tr>
<td>sdm-high-8</td>
<td>$256 \times 256 \times 400$</td>
<td>25</td>
<td>10</td>
<td>0.25/0.025/0.25/1.0/0.5</td>
<td>$1.3 \times 10^{-9}$</td>
</tr>
<tr>
<td>sdm-high-32</td>
<td>$256 \times 256 \times 400$</td>
<td>25</td>
<td>10</td>
<td>0.20/0.020/0.20/1.0/0.2</td>
<td>$5.1 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

Table 1 includes the run label (bulk or SDM microphysics), grid resolution (coarse, middle, or high), and SDND (8, 32, 128, or 512). The grid resolution corresponds to a quarter of the domain from the original RICO setup (i.e., gridbox size of $100 \times 100 \times 40$ m$^3$ with $64 \times 64 \times 100$ grid points); the middle and high resolutions denote settings resulting in halved and quartered gridbox dimensions, respectively (with the domain size kept constant). For each simulation, there are five time steps defined: long and short time step of the Eulerian component (the short one used for sound-wave terms), the time step used for integrating the condensational growth/evaporation equation, the time step used for solving collisional growth using the Monte Carlo scheme, and the time step for integration of particle motion equations. The last column lists mean superdroplet number densities per volume.

4. Results: Cloud microstructure

Figures 2–4 present height-resolved statistics of supersaturation ($S$), cloud droplet concentration (CDNC), droplet effective radius ($r_{eff} = \langle r^3 \rangle / \langle r^2 \rangle$), liquid water content (LWC), cubed ratio of mean volume radius to effective radius ($k = \langle r^3 \rangle / r_{eff}^3$), and standard deviation of cloud droplet radius ($\sigma = (r^2 - \langle r^2 \rangle)^{1/2}$). The analysis is constrained to grid cells with CDNC $> 20$ cm$^{-3}$. All size spectrum features are derived for SDs representing particles of radius between 1 and 24 μm. The same CDNC threshold and radius range was used in Arbabs et al. (2009) and both correspond to characteristics of the Fast-FSSP. The analysis is restricted to the last 4 h of the simulations and is based on SD data (particle positions and sizes) output every 10 min of simulated time.

The plot construction method was chosen following the methodology of Arbabs et al. (2009) and Figs. 2–4 are intended for comparison with their Figs. 1 and 2. For
convenience, selected data from Arabas et al. (2009, their Figs. 1 and 2) are presented in Fig. 5. In the present analysis, for each level of the model grid and each plotted parameter a list of values matching the in-cloud criterion is constructed, sorted, and linearly interpolated to find the 5th, 25th, 45th, 55th, 75th, and 95th percentiles. Levels with less than 0.05 \( N_{\text{max}} \) data points, where \( N_{\text{max}} \) is the number of data points at the level with the highest number of data points, are discarded from the analysis. The 5th–95th percentile, the interquartile, and the 45th–55th percentile ranges are plotted as a function of height using red, green, and blue bars, respectively. Profiles composed of the 45th–55th percentile range bars are referred to as median profiles.

The vertical extent of circa 10 m of the Fast-FSSP sample volume (assuming 10-Hz sampled dataset as used in Arabas et al. (2009)) is comparable to the gridcell sizes used in the simulations. However, the gridcell volumes on the order of \( 10^3 \)–\( 10^5 \) m\(^3\) are incomparable with the Fast-FSSP sample volume of \( 10^{-6} \) m\(^3\)—something one has to bear in mind when comparing the SDM results with Fast-FSSP observations. Furthermore, the employed simulation setup is a composite case representing typical conditions rather than a particular day of the RICO campaign.

**a. Supersaturation**

The profiles of supersaturation, especially for the high and middle resolutions, show the characteristic cloud-base maximum confirming that the model formulation and time resolution allows us to capture the influence of CCN activation kinetics on the evolution of supersaturation. The values of both the maximal
supersaturation (~1%) and a roughly estimated supersaturation relaxation time (about 100 s assuming about 1 m s⁻¹ vertical velocity, and an approximately 100-m height scale over which the supersaturation falls off to an asymptotic value) correspond to those reported in modeling studies employing supersaturation-predicting models (e.g., Morrison and Grabowski 2008; Khvorostyanov and Curry 2008). Comparison of the supersaturation values predicted by the model with measurements is not viable as direct measurements of supersaturation in clouds are virtually unavailable (Korolev and Mazin 2003).

It is worth noting here that one of the strengths of the Lagrangian particle-based approach for representing water condensate in simulations of clouds is the inhibition of spurious production of cloud-edge supersaturation inherent in Eulerian models (Andrejczuk et al. 2008, their paragraph 10 and references therein).

b. Droplet concentration

The range of drop concentration values depicted in Figs. 2–4 falls within the range of CDNC values observed during RICO and presented in Arabas et al.
Profiles based on data from model runs with SDND of 32, 128, and 512 exhibit little variability of CDNC with height with a slight increase in values toward the top of the cloud field, which is in accord with RICO observations. The discrepancies in the median values and the spread of CDNC among different model runs show, however, that the prediction of drop concentration is sensitive to the choice of SDND.

c. Effective radius

The effective radius profiles are robust to both grid and SDND choices, and they do resemble the profiles depicted in Arabas et al. (2009, their Fig. 2; Fig. 5). The profiles show a gradual increase from the cloud base up to the altitude of 700–800 m where the median values of $r_{eff}$ reach 15–20 μm. Above, the profiles differ more from one model run to another, but the flattening of the $r_{eff}$ profile slope is a robust feature. The reduced slope of the median profiles of $r_{eff}$ reflects (i) the chosen 1–24-μm drop radius range; (ii) the decreased efficiency, in terms of radius change, of the condensational growth for larger droplets; and (iii) the increased efficiency of drop collisions reached after the initial condensational growth stage [see, e.g., Zhang et al. (2011, their section 3.1) for discussion of influence of precipitation on effective radius profiles].

d. Liquid water content

LWC profiles depicted in Figs. 2–4 show significant spread of values at a given level. This is in accord with

Fig. 3. As in Fig. 2, but for model runs sdm-coarse-32, sdm-middle-32, and sdm-high-32.
RICO observations and suggests mixing-induced dilution of cloud and the resultant decrease of water content [cf. the discussion of the adiabatic fraction profiles in Arabas et al. (2009, their Fig. 2)]. In SDM the condensational growth and evaporation is computed using values of supersaturation interpolated to SD positions, hence the mixing scenario is not homogeneous as different droplets are exposed to different supersaturation within a single grid cell.

The decrease in LWC in the upper part of the cloud field is correlated with an increase of rainwater mixing ratio (not shown). In the lower part of the cloud field, the median profiles of LWC obtained in the simulation with middle and high grid resolution show arguably reasonable agreement with LWC profiles derived from RICO observations depicted in van Zanten et al. (2011, their Fig. 8), Gerber et al. (2008, their Fig. 1), and Abel and Shipway (2007, their Fig. 7), taking into account that the referenced observations were performed with different instruments having different sampling rates and spectral ranges.

e. The k coefficient

The cubed ratio of the mean volume radius to the effective radius has been used to parameterize the cloud droplet spectrum width when representing the first aerosol indirect effect in general circulation and climate models (Brenguier et al. 2000). Brenguier et al. (2011) reported that characteristic values of the k coefficient derived from RICO Fast-FSSP measurements were
approximately 0.8 ± 0.1 (their Table 4 and Figs. 4 and 6). The model-predicted median values of $k$ fall within this range only for simulations with SDND of 128 and 512. Simulations with SDND of 8 predict values of $k$ hardly different from unity—an asymptotic value characterizing monodisperse droplet population (single SD within the Fast-FSSP size range).

f. Drop radius standard deviation

Consistent with the behavior of the coefficient $k$ for low SDND, $\sigma_r$ hardly differs from zero when SDND of 8 is used (a bias-uncorrected estimator for $\sigma_r$ is used). For simulations in Fig. 4 the 5th percentile of $\sigma_r$ is greater than zero at all levels, and the profile shape is robust to increase of SDND from 128 to 512. Values of $\sigma_r$ for simulations with SDND of 128 and 512 range from 1 to 6 $\mu$m. The model thus roughly matches, yet generally underestimates, the range of values found in RICO observations reported in Arabas et al. (2009, their Fig. 1; Fig. 5). It is worth noting here that the measurements of cloud droplet spectral width are subject to several uncertainties contributing to artificial broadening of the measured size spectrum [Brenguier et al. (1998), their section 4 and references therein]. While the design of the Fast-FSSP instrument addresses these issues, some inherent limitations of these measurements may in principle still lead to potential overestimation of the measured values of $\sigma_r$.

The model-predicted values of $\sigma_r$ are larger than those obtainable in adiabatic drop growth process (Yum and Hudson 2005), suggesting that the model does capture to some extent the mixing-induced broadening of the cloud droplet spectrum.

5. Results: Precipitation microstructure

Analysis presented in Fig. 6 is intended for comparison with Baker et al. (2009, their Fig. 4) based on RICO observations using the 2D-S instrument and classifying particles into 61 size bins spanning the 2.5–1500–$\mu$m size range in radius. In Baker et al. (2009) a mean size spectrum was derived from measurements within rain shafts below the cloud base at an altitude of 600 ft (~183 m). To derive comparable quantities from the simulation results, the SDs in each grid cell were classified into size bins of the same layout as used by the 2D-S instrument, an altitude range of 600–330 ft was chosen, and only grid cells with rainwater mixing ratio $q_r > 0.001$ g kg$^{-1}$ were taken into account.

Comparison of Fig. 6 with Baker et al. (2009), their Fig. 4; see also the gray line in the background of Fig. 6) reveals fair agreement with the measurements for drop diameters greater than 500 $\mu$m regardless of the grid resolution or SDND choice. The spectra from the simulation with highest SDNDs resemble most closely the measurements having the lowest concentrations in the 100–400–$\mu$m-diameter range. This is despite the coarse grid setting, which implies that the modeled precipitation size spectrum is more sensitive to the model spectral resolution than to the spatial resolution within the range of settings explored in this study. The growing sensitivity of the results to SDND with growing particle size in the 10–100–$\mu$m range was also depicted in Riechelmann et al. (2012, their Fig. 8b, plotted as a function of particle radius; diameters used herein).

All simulations disagree markedly with the measurements within the 10–20–$\mu$m-diameter range where the
2D-S probe measured “most likely deliquesced aerosols” (Baker et al. 2009). The drop breakup process was identified in Baker et al. (2009) as another possible source of droplets smaller than 100 μm. However, neither the drop breakup nor aerosol sources are represented in the model.

6. Summary

The macrophysical features of the simulated cloud field do not show convergence with respect to grid resolution, which was also noted in previously published results from LES sensitivity studies using the same simulation setup. In general, the sensitivity of liquid and rainwater path and the cloud cover to the grid resolution is more pronounced than the sensitivity to the spectral resolution of the simulations.

The idealized nature of the employed modeling setup as well as the discussed inherent limitations of the simulations and the measurements still makes their comparison qualitative rather than quantitative. Yet, the reasonable agreement of the presented simulated cloud microphysical parameters with previously published data derived from in situ measurements suggests that the set of processes represented in SDM includes at least the key players involved in determining the features of the size spectra of cloud and precipitation particles.

What militates in favor of pertinence of the obtained results is that SDM employs fewer parameterizations in comparison with bulk or bin models to describe processes occurring at the microscale. In particular, SDM makes explicit use of the Köhler curve and aerosol size spectrum shapes as opposed to employment of parameters such as the exponent in Twomey’s formula for CCN activation parameterization in bin models or the autoconversion threshold in Kessler-type bulk models. This results in improved traceability of the cloud and precipitation microphysical properties to the ambient aerosol characteristics.

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Fig. 6. Comparison of model-predicted spectra for particles within size range of the 2D-S instrument, within grid cells with \( q_r > 0.001 \) g kg\(^{-1} \) and within an altitude range of 600 ± 330 ft. Figure intended for comparison with Baker et al. (2009, their Fig. 4) (both plots share the same axes ranges; the gray line in the background of the plot herein is the digitized mean distribution from the referenced paper). See section 5 herein for details.
REFERENCES


