Cloud droplet diffusional growth in homogeneous isotropic turbulence: bin microphysics versus Lagrangian superdroplet simulations

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Abstract. Increase of the spectral width of initially monodisperse population of cloud droplets in homogeneous isotropic turbulence is investigated by applying a finite-difference fluid flow model combined with either Eulerian bin microphysics or Lagrangian particle-based scheme.

15 The turbulence is forced applying a variant of the so-called linear forcing method that maintains the mean turbulent kinetic energy (TKE) and the TKE partitioning between velocity components. The latter is important for maintaining the quasi-steady forcing of the supersaturation fluctuations that drive the increase of the spectral width. We apply a large computational domain, 64^3 m^3, one of the domains considered in Thomas et al. (2020). The simulations apply 1 m grid

20 length and are in the spirit of the implicit large eddy simulation (ILES), that is, with small-scale dissipation provided by the model numerics. This is in contrast to the scaled-up direct numerical simulation (DNS) applied in Thomas et al. (2020). Two TKE intensities and three different droplet concentrations are considered. Analytic solutions derived in Sardina et al. (2015), valid for the case when the turbulence integral time scale is much larger than the droplet phase

25 relaxation time scale, are used to guide the comparison between the two microphysics simulation techniques. The Lagrangian approach reproduces the scalings relatively well. Representing the spectral width increase in time is more challenging for the bin microphysics because appropriately high resolution in the bin space is needed. The bin width of 0.5 μm is only sufficient for the lowest droplet concentration, 26 cm^{-3}. For the highest droplet concentration,

30 650 cm^{-3}, an order of magnitude smaller bin size is barely sufficient. The scalings are not expected to be valid for the lowest droplet concentration and the high TKE case, and the two

microphysics schemes represent similar departures. Finally, because the fluid flow is the same for all simulations featuring either low or high TKE, one can compare point-by-point simulation results. Such a comparison shows very close temperature and water vapor point-by-point values across the computational domain, and larger differences between simulated mean droplet radii and spectral width. The latter are explained by fundamental differences in the two simulation methodologies, numerical diffusion in the Eulerian bin approach and relatively small number of Lagrangian particles that are used in the particle-based microphysics.

1 Introduction

Cloud droplet spectra in natural ice-free clouds significantly affect such key processes as drizzle/rain formation and transfer of solar radiation through the cloudy atmosphere. At the same time, modeling of droplet spectra is cumbersome and thus simplified approaches are often used, such as the bulk microphysics where the shape of the droplet spectrum is prescribed or not considered at all. When simulation of the droplet spectral shape is required, there are two basic modeling methodologies that can be used. The first one is a traditional bin approach where the Eulerian continuous in space and time spectral density function is used. In its numerical implementation, the spectral density function is represented by a finite number of radius (or mass) bins. Each bin is advected in the physical space and all bins are combined at model grid locations to calculate the change of the spectral density function due to droplet growth. The bin microphysics is a well-established approach to modeling droplet spectral evolution, see Khain et al. (2015) and references therein. The second approach represents the multiphase nature of real clouds by applying Lagrangian point particles. Each particle represents an ensemble of natural droplets with the same properties, it is advected by the simulated air flow, and it grows in response to local conditions. The Lagrangian approach, often referred to as the super-droplet method (Shima et al., 2009), is a relatively novel modeling technique that gains popularity in cloud modeling because of its fidelity, especially for the simulation of aerosol-cloud interactions (e.g., Andrejczuk et al., 2008; Shima et al., 2009; Riechelmann et al., 2012; Arabas and Shima, 2013; Unterstrasser et al., 2017; Hoffmann et al., 2019; Dziekan et al., 2019; see also Grabowski

et al., 2019). The Lagrangian approach is referred to as the "swarm model" in the astrophysical context (see Li et al., 2017 and references therein).

65   The two methodologies have their inherent limitations. The bin microphysics is affected by the numerical diffusion as any Eulerian approach. Advection of bins in the physical space typically leads to unavoidable numerical spreading of regions with rapid droplet spectral changes, for instance, near cloud edges. The diffusional growth of cloud droplets is represented by the advection of the spectral density function in the radius (or mass) space and it is impacted by

70   numerical aspects similar to the advection in the physical space (e.g., section 3.1 in Li et al., 2017). The combined effect of the advection in the physical space and advection in the radius space is argued by Morrison et al. (2018) to result in artificial broadening of the droplet spectra in cloud simulations applying bin microphysics. For the Lagrangian microphysics, an obvious limitation is the limited and usually small number of Lagrangian particles that can be afforded in

75   realistic cloud simulations, especially considering an enormous number of cloud and precipitation particles in natural clouds. However, the Lagrangian methodology has clear benefits when compared to the bin scheme. These include the lack of numerical diffusion, realistic representation of the stochastic nature of the cloud droplet growth, possibility of including physically-based representation of the unresolved scales impact on droplet growth (i.e.,

80   allowing the multiscale simulation of a turbulent cloud), and providing a better framework for aerosol-cloud interactions and representation of ice processes. Grabowski et al. (2019) provide a review of these benefits.

     Grabowski (2020a, 2020b; G20a and G20b, respectively) compared cloud droplet activation and

85   growth by the diffusion of water vapor in simulations of a laboratory cloud chamber and a single cumulus congestus cloud, respectively. The laboratory cloud chamber at the Michigan Technological University (see http://phy.sites.mtu.edu/cloudchamber/) forms a cloud because of the temperature and humidity differences between lower and upper horizontal boundaries that drive turbulent Rayleigh–Bénard convection. G20a shows a good agreement between droplet

90   spectra predicted by the two methodologies when averaged over the chamber volume away from boundaries. G20a argued that the good agreement was because of the constant chamber pressure assumed in the simulations. This agrees with Morrison et al. (2018) conjecture that the artificial

spectral broadening comes from the coupling between vertical advection in a stratified environment (that provides the supersaturation source) and advection in the bin space that represents response of the droplet population to the supersaturation forcing. Cumulus congestus case from G20b is based on a modeling study by Lasher-Trapp et al. (2005) that considered a cloud observed by a radar and an instrumented aircraft during the Small Cumulus Microphysics Study (SCMS) near Cape Canaveral, Florida, during July–August of 1995. A unique aspect of the G20b study is application of the piggybacking methodology. Piggybacking refers to using two microphysics schemes in a single cloud simulation, one scheme driving the dynamics and the other one piggybacking the simulated flow, see Grabowski (2019) for a review. Operating the two schemes in the same cloud-scale flow allows point-by-point comparison of droplet spectra predicted by the two schemes. A significantly larger mean spectral width simulated by the bin scheme across the entire cloud depth is the largest difference between the two schemes in G20b simulations.

In this paper, we discuss differences between the two methodologies for representing droplet spectral evolution in numerical homogeneous isotropic turbulence. Li et al. (2017) present similar comparisons applying dynamic and kinematic simulations, and including collision-coalescence. Here, we consider diffusional growth of cloud droplets only. The direct numerical simulation (DNS) methodology (e.g., Vaillancourt et al., 2001, 2002; Lanotte et al., 2009; Li et al., 2019) and scaled-up DNS technique (Thomas et al., 2020) allow representation of turbulence impact on the droplet spectral width with an unprecedented fidelity. Sardina et al. (2015) and Grabowski and Abade (2017) provide stochastic model reference for such studies (cf. Fig. 10 in Thomas et al., 2020). In contrast to Thomas et al. (2020) who used a traditional spectral DNS code, we apply a finite-difference fluid flow model that does not require small-scale dissipation to maintain computational stability. It follows that the simulations are in the spirit of the implicit large eddy simulation (ILES) where the model numerics provide the required small-scale dissipation of the turbulent kinetic energy (TKE) and scalar variance. Details of the fluid flow model are presented in the next section with the emphasis on the forcing to maintain the quasi-steady turbulence, the key element of the homogeneous isotropic turbulence DNS. Two turbulence cases are considered, the low TKE case (following Lanotte et al., 2009 and Thomas et al., 2020) and the high TKE case, the latter featuring hundred times larger TKE than the former.

Section 3 introduces the temperature and water vapor equations for moist simulations and presents results from simulations without droplets. Section 4 introduces numerical representation of cloud droplets applying either Eulerian bin microphysics or Lagrangian superdroplets. Results of simulations with droplets are presented in section 5 focusing on the ability of either scheme to represent theoretical scalings derived by Sardina et al. (2015) and on the comparison of the droplet spectra simulated by the two schemes. Section 6 shows grid-volume by grid-volume comparison of model results facilitated by the simulation methodology, exposing additional limitations of the two microphysics simulation approaches. A brief summary in section 7 concludes the paper.

2 Homogeneous isotropic turbulence simulations

2.1 The model and model forcing

The EULerian--semi-LAGrangian (EULAG) anelastic finite-difference fluid flow model (http://www.mmm.ucar.edu/eulag/) is used in this study in the ILES mode (Margolin and Rider, 2002; Andrejczuk et al., 2004; Margolin et al., 2006; Grinstein et al., 2007). ILES implies that the model uses no explicit dissipation and removes small-scale velocity and scalar fluctuations through numerical diffusion provided by the monotone advection scheme. The fluid flow equations for homogeneous isotropic turbulence simulations are (e.g., Lanotte et al., 2009, Li et al., 2017):

$$\frac{\partial \boldsymbol{u}}{\partial t} + \text{div}\,(\boldsymbol{u}.\boldsymbol{u}) = -1/\rho \,\text{grad}\,p + \boldsymbol{f} \qquad (1)$$

$$\text{div}\,\boldsymbol{u} = 0, \qquad\qquad (2)$$

where $\boldsymbol{u}$ is the fluid flow velocity, p is pressure, $\rho = 1$ kg m^{-3} is the air density, and $\boldsymbol{f}$ is the turbulence forcing term. The forcing term ensures that the turbulence is maintained throughout the simulation with TKE flowing from large-scales towards the small-scale dissipation. The traditional technique to force the quasi-equilibrium homogeneous isotropic turbulence,

155   convenient for spectral models, is to consider the forcing only for a few low-wavenumber modes. However, such an approach is not practical for the finite-difference model used here. Instead, we apply a method in the spirit of the so-called linear forcing of Rosales and Meneveau (2005) and Onishi et al. (2011). In the homogeneous isotropic turbulence, TKE increases with the eddy size L as $L^{2/3}$, that is, TKE is dominated by contributions from the largest eddies. Hence, one can

160   force the turbulence by simply ensuring that the TKE does not change from one model time step to the next one because such forcing affects mostly large eddies. This implies that $\boldsymbol{u}^{(n+1)} = \alpha \, \boldsymbol{u}^{(n)}$ with $\alpha = (E_t/E^{(n)})^{1/2}$, where n and $n+1$ represent time levels, $E^{(n)}$ is TKE at the n time level, and E_t is the target TKE (see Eq. 3 in Onishi et al., 2011). The finite difference representation of such a forcing is given by

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$$\boldsymbol{f} = (\boldsymbol{u}^{(n+1)} - \boldsymbol{u}^{(n)})/\Delta t = \boldsymbol{u}^{(n)}(\alpha\text{-}1) \, / \, \Delta t \ , \quad (3)$$

that is, as in the case of the linear forcing of Rosales and Meneveau (2005). The TKE dissipation rate ε can be derived assuming that the TKE does not change in time [see (5) in Onishi et al.,

170   (2011)] as

$$\varepsilon = 2 \, E_t \, (\alpha\text{-}1) \, / \, \Delta t \ . \quad (4).$$

Eq. 4 is particularly useful in ILES because it allows diagnosing the TKE dissipation rate that is

175   otherwise not known.

The forcing described above was initially applied in dry ILES simulations, that is, the EULAG model solving (1) and (2). For those tests (and for other simulations described in this paper), the initial flow field (scaled-up to approximately match the required TKE) was taken as the initial

180   flow pattern in decaying turbulence simulations in Andrejczuk et al. (2004), see Fig. 1 therein. Other parameters of the test simulations correspond to low TKE setup as described in the next section. Those initial tests forced as in (3) revealed the need for additional forcing modifications as discussed below.

185   As in other studies of forced homogeneous isotropic turbulence (e.g., Lanotte et al., 2009), the model applies computational domain with triply-periodic lateral boundary conditions. Such boundary conditions together with (2) imply that the mean flow across the domain has to be uniform. For instance, $\mathrm{d}<u_z>_{xy}/\mathrm{d}z$ (where u_z is the vertical velocity and $<.>_{xy}$ is the horizontal average) has to vanish, and the same is true for the other two spatial directions. However, the

190   vertically-uniform $<u_z>_{xy}$ can evolve in time. In the initial tests, a gradual development of the mean flow across the domain was noticed. In other words, in addition to driving the turbulence inside the computational domain, the forcing (3) resulted in a gradual development of the mean flow across the domain. To eliminate this undesirable behavior, an additional forcing term is included in the model equations that controls the mean flow across the domain. The additional

195   forcing term is a simple relaxation towards the vanishing mean flow, that is,

$$f = (-<u_x>/\tau, \ -<u_y>/\tau, \ -<u_z>/\tau \ ), \qquad (5)$$

where $\boldsymbol{u} = (u_x, u_y, u_z)$, $<.>$ is the 3D average, and τ is the relaxation time scale taken as 10 model

200   time steps. Note that (5) does not dump the flow perturbations, but only prevents the mean flow development. In simulations presented here, the mean flow across the domain after applying (5) was limited to about 10^{-16} m s^{-1}.

Second, although (3) maintains the mean TKE, the TKE partitioning between the three velocity

205   components is allowed to evolve. As a result, the magnitude of the root mean square (rms) vertical velocity can vary in time and affect supersaturation fluctuations and droplet growth. Thus, (3) needs to be modified to maintain the uniform TKE partitioning between the three components. The idea is to apply the forcing for each component separately and assuming equipartition of the TKE between all three components. For instance, for the x velocity

210   component, u_x, the modified forcing should be $u_x^{(n+1)} = \alpha_x \, u_x^{(n)}$ with $\alpha_x = [2 \, E_t / 3 \, <u_x^{(n) \, 2}>]^{1/2}$, where, as before, E_t is the target TKE. The forcing term for u_x is then given by:

$$f_x = u_x^{(n)}(\alpha_x - 1) / \Delta t \ , \qquad (6)$$

215   and similar for the two other velocity components.

To document the necessity of using the more elaborate approach (6), two simulations applying either (3) combined with (5) or (6) combined with (5) were run (details of the simulations are provided in the next section). Figure 1 compares TKE and rms vertical velocity in the two simulations. The figure shows that the modified forcing, that is, applying (6) in place of (3), maintains not only the TKE, but also a uniform in time rms vertical velocity. The latter implies even partitioning of the TKE between the velocity components in agreement with the forcing formulation. The fluctuating in time rms vertical velocity in simulations applying forcing (3) leads to evolving supersaturation standard deviation in moist simulations and thus more complex mean droplet size evolution (not shown). In summary, the forcing term driving the isotropic homogeneous turbulence applied in this study is the sum of (5) and (6).
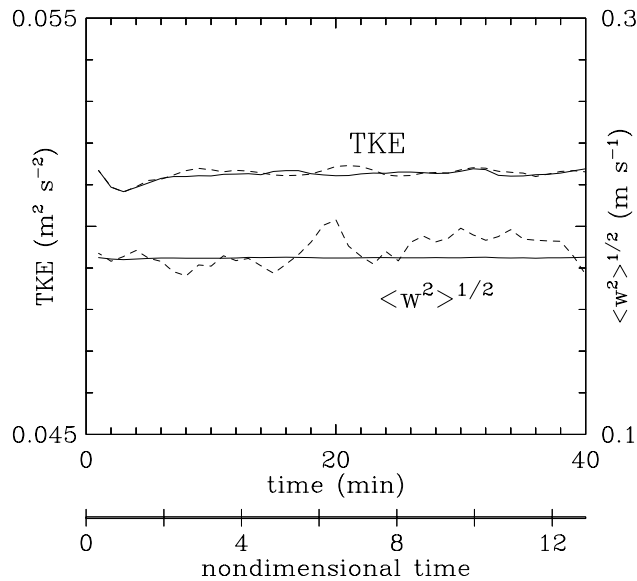
Figure 1. Evolutions of the TKE and rms vertical velocity in low TKE simulations applying either (3) – dashed lines, or (6) – solid lines, as part of the forcing. The nondimensional time is the time divided by the turbulence integral time, 187 sec for the low TKE simulations.

2.1 The setup of dynamic simulations

The triply-periodic computational domain is 64^3 m^3 with the model grid length of 1 m. This is one of the domains considered in Thomas et al. (2020) and close to the turbulent rising parcel extent of 50 m considered in Grabowski and Abade (2017). Such a domain size is also similar to the grid volume of LES simulations of natural clouds (e.g., Siebesma et al., 2003, Stevens et al., 2005, VanZanten et al., 2011). For the fluid flow, we consider two turbulence intensities as expressed by the prescribed TKE. The "low TKE" simulations assume the TKE of 5.2 x 10^{-2} m^2 s^{-2}. Such a TKE corresponds to the TKE dissipation rate of 10^{-3} m^2 s^{-3} in 64^3 m^3 scaled-up DNS simulations in Thomas et al. (2020) that followed DNS simulations in Lanotte et al. (2009). The low TKE setup corresponds to the rms vertical velocity around 0.2 m s^{-1} (see Fig. 1), evolving maximum vertical velocity between 0.5 and 0.8 m s^{-1}, and integral time scale (see Eq. 7 in Grabowski and Abade, 2017) of 187 sec, or about 3 minutes. The model time step for the low TKE simulations dictated by the CFL stability criterium is $\Delta t = 0.25$ sec. The low TKE dry dynamics simulations (i.e., solving only Eqs. 1 and 2 only) and simulations without droplets (section 3) were run for 40 minutes (around 12 integral time scales as shown in Fig. 1). Simulations with droplets discussed in section 5 were run for 20 min or about 6 integral time scales starting from minute 28 of 40-min simulations presented in the next section. The "high TKE" simulations consider hundred times larger TKE, i.e., 5.2 m^2 s^{-2}. High TKE simulations feature ten times larger rms and maximum velocities (i.e., around 2 m s^{-1} and 5 to 8 m s^{-1}, respectively) together with ten times smaller integral time scale of about 19 sec. Model time step in high TKE simulations was proportionally reduced to 0.025 sec. The high TKE simulations were run for the same number of time steps as the low TKE simulations, that is, for the total time of either 4 or 2 minutes, that is, either 12 or 6 integral time scales. Model data were saved every 15/1.5 sec for low/high TKE simulations and they are used in the analysis presented here.

Eq. 4 allows estimation of the TKE dissipation rate. The parameter α in the forcing term is monitored from time step to time step during the simulations. The typical value in both low and high TKE is α-1 $\approx$ 2 x 10^{-4}. With the target TKE $E_t = 5.2$ x 10^{-2} m^2 s^{-2} and $\Delta t = 0.25$ sec in low TKE simulations, the TKE dissipation diagnosed from (4) is $\varepsilon \approx 4$ x 10^{-4} m^2 s^{-3}. This value approximately agrees with the assumed low TKE turbulence simulation setup. For the high TKE, the target TKE and the model time step imply $\varepsilon \approx 4$ x 10^{-1} m^2 s^{-3}. This is a rather extreme TKE

dissipation rate for small cumulus dynamics (e.g., Siebert et al., 2006), but perhaps not unusual

270   for deep convection as simulated, for example, by Benmoshe et al. (2012).

Figure 1, already mentioned in section 2a, documents TKE evolution together with the rms vertical velocity in the low TKE simulation. The horizontal axis shows either the real time or the nondimensional time using the integral time scale. As the figure shows, the forcing maintains the

275   TKE and rms vertical velocity as expected by the forcing design. Figure 2 shows the TKE spectra for low and high TKE at the minute 28/2.8 that are used as initial conditions for moist simulations with droplets. The spectra have a classical shape characteristic of a relatively low-Reynolds-number homogeneous isotropic numerical turbulence (e.g., Fig. 2 in Rosales and Meneveau, 2005). Spectra at different times are similar to those in Fig. 2 (not shown).

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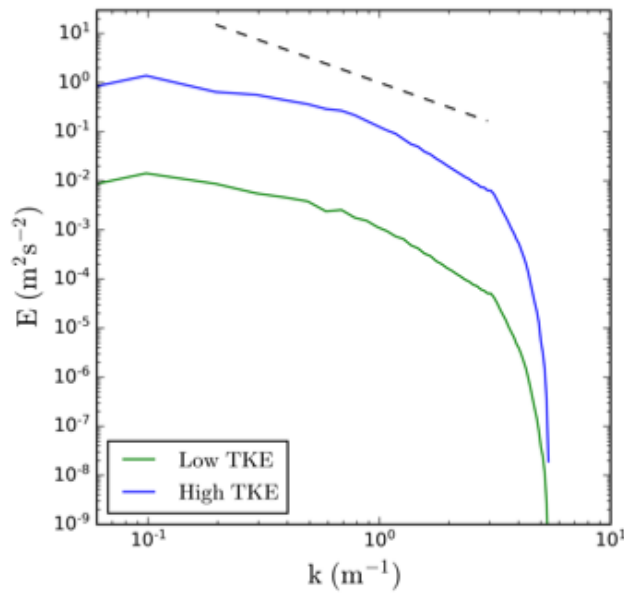
Figure 2. Energy spectra for the fluid flow simulations without droplets at minute 28/2.8 for low/high TKE simulation without droplets. The dashed line represents the -5/3 Kolmogorov slope.

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The turbulence dynamics in moist simulations described in the next section is exactly as described above, that is, the impact of cloud droplets and of the latent heating on the flow is neglected. This is because the air density is assumed constant and the flow equations exclude the buoyancy term as typical in the homogeneous isotropic DNS simulations (see, for instance, eq. 1

290   in Lanotte et al., 2009). Because the flow is exactly the same in all simulations, one can compare model results grid volume by grid volume as in the piggybacking methodology (Grabowski, 2019 and references therein). This allows a comprehensive comparison of simulation results as illustrated in section 6.

295   **3 Thermodynamics in ILES moist simulations**

In addition to the momentum, the moist ILES of homogeneous isotropic turbulence solves the temperature T and water vapor mixing ratio q_v equations in the form:

300      $\partial T/\partial t + \text{div}\,(\boldsymbol{u}\,T) = L_v/c_p\,C_d - g/c_p\,u_z$,   (7)

$\partial q_v/\partial t + \text{div}\,(\boldsymbol{u}\,q_v) = -\,C_d$,   (8)

where $L_v = 2.5 \times 10^6$ J kg^{-1} is the latent heat of condensation, $c_p = 1015$ J kg^{-1} K^{-1} is the specific
305   heat of air at constant pressure, g $= 9.81$ m s^{-2} is the gravitational acceleration, and C_d is the condensation rate, the rate of change of the cloud water mixing ratio resulting from the diffusional growth of cloud droplets. Calculation of the condensation rate depends on the microphysics scheme as explained below.

310   In the spirit of DNS studies of homogeneous isotropic turbulence, the initial temperature and water vapor mixing ratio in moist simulations are assumed spatially uniform. The actual values are taken as in Thomas et al. (2020), that is, $T = 283$ K and q_v at saturation assuming environmental pressure of 1000 hPa. The spatially-uniform initial conditions justify the triply-periodic computational domain. The last term in (6) represents the temperature change due to
315   adiabatic air expansion resulting from the vertical motion in the stratified environment. This term drives small-scale supersaturation fluctuations in the otherwise uniform environment; see discussion in section 3 in Vaillancourt et al. (2001). Such a modeling framework is a simplification of a truly stratified environment where the environmental temperature and pressure are functions of height and typically the potential temperature (an invariant for dry
320   adiabatic vertical displacements) rather than the temperature is applied as the model variable. In

some DNS studies, the temperature and moisture equations are combined into the supersaturation equation that includes the source due to the vertical motion (as the last term in Eq. 6) and the sink due to droplet growth, Eq. (2) in Lanotte et al. (2009) or Eq. (2) in Sardina et al. (2015); see Eq. (10) below.

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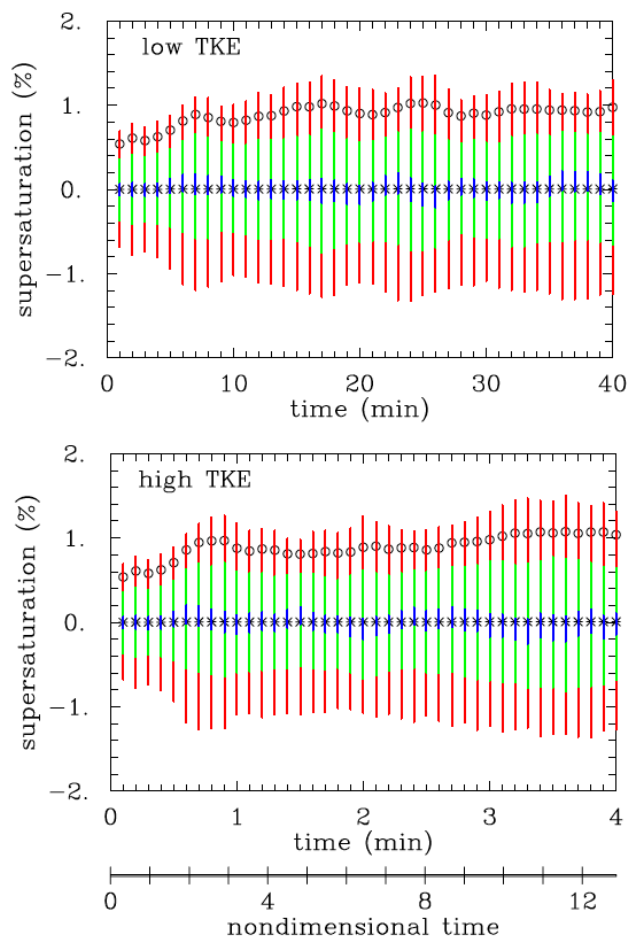
Figure 3. Evolution of the supersaturation spatial distribution statistics for a 40-minute low TKE (upper panel) and high TKE (lower panel) moist simulations without droplets. Stars and circles show the mean and standard deviation of the spatial distribution, respectively. The extent of the color bars shows the percentiles of the distribution: red is for 10-90th percentile, green is for 25-75th percentile, and blue is for 45-55th percentile. The nondimensional time, the same for low and high TKE, is shown below the lower panel.

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The initial test of the moist ILES framework considers a 40-min long low TKE and 4-min long high TKE simulations without droplets (i.e., both up to about 12 integral time scales) and

335   initiated in the same way as the dry simulation illustrated in Figs. 1 and 2. The simulations apply the fluid flow as described above and solving (7) and (8) without the condensation term C_d. In

such simulations, the largest temperature change is possible when the air parcel rises across the entire computational domain depth, that is, 64 m, with the corresponding temperature change of about 0.64 K as given by (7). Such a maximum temperature change leads to the supersaturation

340   change from the initial zero to about 4%. In the numerical simulation, the maximum temperature deviations from the uniform initial 283 K are typically smaller than 0.5 K. The evolutions of supersaturation statistics are shown in Fig. 3. Despite the dramatic difference in the TKE levels, the statistics are similar regardless of the TKE level, in agreement with the parcel argument. Only after including the source due to condensation, the evolutions become different depending

345   on the droplet characteristics and the TKE level. Small differences in the evolutions in Fig. 3 come from different flow realizations between low and high TKE cases.

4 ILES moist simulations with droplets

350   The general microphysical setup considers initially monodisperse population of cloud droplets with the radius of 13 μm present in three different concentrations: 26, 130, and 650 cm^{-3}. The concentration 130 cm^{-3} was considered in Lanotte et al. (2009) and Thomas et al. (2020) and it corresponds to the mean cloud water content of about 1.2 g m^{-3}. In addition, the five-times smaller and five-times larger droplet concentrations are considered to document how the two

355   microphysics schemes represent the expected scalings. The mean cloud water content in simulations with the increased (decreased) droplet concentration is about 6.0 (0.24) g m^{-3}. Moist simulations with droplets start at minute 28 of the moist simulation without droplets, that is, applying the flow field analyzed in Fig. 2, together with the temperature and moisture field at minute 28 in Fig. 3. The simulations are run for additional 20 minutes for the low TKE setup,

360   saving data every 15 sec. The high TKE simulations are run for 2 minutes and the data are saved every 1.5 sec. The data are used in the analysis of both macrophysical (e.g., the supersaturation characteristics) and microphysical (e.g., droplet spectra) simulated by the two microphysics schemes. Sardina et al. (2015) derived scalings for the case when the droplet phase relaxation time is much shorter than the turbulence integral time scale. This is the case for the selected

365   domain size and the low TKE for all droplet concentrations. For the high TKE and low droplet concentration (i.e., 26 cm^{-3}), the phase relaxation time (about 10 seconds) is the closest to the

turbulence integral time scale (about 19 seconds), so some deviations from the theoretical scaling should be expected as shown below.

4.1 Lagrangian and Eulerian microphysics schemes

The particle-based Lagrangian scheme considers on average 40 Lagrangian particles (superdroplets) per grid volume, each featuring the initial radius of 13 μm. The number of superdroplets per grid volume together with the assumed droplet concentration dictates the multiplicity that is assumed the same for all superdroplets. Although the average number of superdroplets per grid volume is small when compared to millions real droplets within a 1 cubic meter grid volume, G20a and G20b document that the number as small as 10 per grid box provides physically-meaningful results; see also Li et al. (2017). At the simulation onset, each superdroplet is placed at a random position within a grid volume. To be consistent with the bin microphysics, superdroplets grow in response to the mean supersaturation predicted inside a grid volume it occupies. Superdroplets are advected applying a model flow field interpolated to the droplet position as in Arabas et al. (2015). The interpolation scheme maintains the incompressibility of the flow at subgrid scales; see discussion of this aspect in section 2.4 in Grabowski et al. (2018). Droplet inertia and droplet sedimentation are not considered. Condensation rate C_d at each time step is calculated by summing up the mass change of all superdroplets present within a given grid volume.

The simulations with superdroplets are referred to as SDS.26, SDS.130, and SDS.650 for droplet concentrations of 26, 130, and 650 cm^{-3}, respectively. The three simulations are completed for both low and high TKE. In addition, a single simulation with 150 superdroplets per grid volume and droplet concentration of 130 cm^{-3} was completed for the low TKE to test the impact of the superdroplet number fluctuations within a grid volume. This simulation is referred to as SDS.HR.130 (HR for high resolution in the radius space).

The Eulerian bin microphysics considers spectral density function represented by 40 equally-spaced bins with the bin size modified in different simulations as described below. The reason for modifications of the bin resolution is to match the results from the Lagrangian microphysics

as shown in the results section. In each bin setup, there is a bin centered at 13 µm that is filled with droplets at the simulation onset. The monodisperse initial droplet size distribution is impossible to be accurately represented using the spectral density function because the monodisperse distribution corresponds to the delta function. However, even with a finite width of the initial distribution, the broadening of the distribution as time progresses (Sardina et al., 2015; Li et al., 2019; Thomas et al., 2020) can be appropriately represented provided that the bin width is appropriately small (see section 5.3). In the bin microphysics, each bin is independently advected in the physical space using the same advection scheme that is applied to the momentum, temperature, and water vapor mixing ratio. Neither droplet sedimentation nor droplet inertia are considered as in the Lagrangian scheme. All bins are combined at each grid volume to calculate evolution of the droplet spectrum due to the local sub- or supersaturation applying a custom-designed 1D advection scheme. The scheme combines the analytic Lagrangian solution of the condensational growth with remapping of the spectral distribution onto the original radius grid using piecewise linear functions (see section 3.2 in Grabowski et al., 2011). As for the Lagrangian scheme, condensation rate C_d at each time step is calculated from the change of the spectral density function due to the droplet growth in each grid volume.

For the low TKE, eight bin simulations with the spectral density function represented by 40 bins and different bin resolutions are considered. The selection of a specific bin resolution is motivated by the results discussed in the next section. The standard bin setup is similar to G20b with a uniform 0.5 µm bin width and 0 to 20 µm bin range. These simulations are BIN.26, BIN.130, and BIN.650 for the three droplet concentrations. The high resolution (HR) simulations have 0.3 µm bin width and the bin layout centered at 13 µm (i.e., from 7 to 19 µm). These simulations are run for 130 and 650 cm^{-3} concentrations and are referred to as BIN.HR.130 and BIN.HR.650, respectively. Very high resolution (VHR) simulations have 0.1 µm bin width, again centered at 13 µm (bin range between 11 and 15 µm) and with 130 and 650 cm^{-3} concentration, BIN.VHR.130 and BIN.VHR.650. Finally, an even higher bin resolution, 0.05 µm bin width and grid centered at 13 µm (i.e., bin range between 12 and 14 µm), is added for the 650 cm^{-3} concentration, BIN.SHR.650 (SHR for Super High Resolution). For the high TKE, only three simulations were completed, BIN.26, BIN.VHR.130, and BIN.VHR.650. Table 1 provides a list of all simulations in both Lagrangian and Eulerian simulations.

Table 1. Details of Lagrangian and Eulerian simulations.

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Lagrangian (superdroplet) simulations:

Low TKE:	SDS.26	26 cm^{-3}, 40 superdroplets per grid volume
	SDS.130	130 cm^{-3}, 40 superdroplets per grid volume
	SDS.HR.130	130 cm^{-3}, 150 superdroplets per grid volume
	SDS.650	650 cm^{-3}, 40 superdroplets per grid volume
High TKE:	SDS.26	26 cm^{-3}, 40 superdroplets per grid volume
	SDS.130	130 cm^{-3}, 40 superdroplets per grid volume
	SDS.650	650 cm^{-3}, 40 superdroplets per grid volume

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Eulerian (bin) simulations:

Low TKE:	BIN.26	26 cm^{-3}, 40 bins centered at 13 μm, 0.5 μm bin width
	BIN.130	130 cm^{-3}, 40 bins centered at 13 μm, 0.5 μm bin width
	BIN.HR.130	130 cm^{-3}, 40 bins centered at 13 μm, 0.3 μm bin width
	BIN.VHR.130	130 cm^{-3}, 40 bins centered at 13 μm, 0.1 μm bin width
	BIN.650	650 cm^{-3}, 40 bins centered at 13 μm, 0.5 μm bin width
	BIN.HR.650	650 cm^{-3}, 40 bins centered at 13 μm, 0.3 μm bin width
	BIN.VHR.650	650 cm^{-3}, 40 bins centered at 13 μm, 0.1 μm bin width
	BIN.SHR.650	650 cm^{-3}, 40 bins centered at 13 μm, 0.05 μm bin width
High TKE:	BIN.26	26 cm^{-3}, 40 bins centered at 13 μm, 0.5 μm bin width
	BIN.VHR.130	130 cm^{-3}, 40 bins centered at 13 μm, 0.1 μm bin width
	BIN.VHR.650	650 cm^{-3}, 40 bins centered at 13 μm, 0.1 μm bin width

445

450

455

460 Droplet growth in both schemes is calculated applying a simplified growth formula as in G20a and G20b:

$$dr/dt = A\,S\,/\,(r+r_0), \quad (9)$$

with A=0.9152 × 10^{-10} m^2 s^{-1} and r_0 = 1.86 μm. The latter is applied to mimic the impact of kinetic effects (Mordy 1959, see Eq. 11 in Clark 1971 or Eq. 2.22 in Kogan 1991). Because of a

465 large mean droplet size, 13 μm, the solution and curvature effects are neglected. The two schemes apply the droplet growth equation (9) in different ways: as a transport (advection) velocity in the Eulerian bin scheme and to calculate individual superdroplet growth in the Lagrangian scheme.

5. Results

470

5.1 Lagrangian microphysics

Figure 4 shows evolutions of the supersaturation standard deviation in low and high TKE
Lagrangian simulations. The supersaturation standard deviation is approximately constant except
475   for the adjustment from initial values in simulations without droplets (cf. Fig. 3). Standard
deviations for the SD.130 and SD.HR.130 simulations are practically the same. Table 2 shows
the standard deviation averaged over the second half of the simulations. When the phase
relaxation time is much smaller than the turbulence integral time scale, the supersaturation
standard deviation is proportional to the product of the rms vertical velocity and the phase
480   relaxation time; $\sigma_S \sim <w^2>^{1/2} \tau_{relax}$, see Sardina et al. (2015). The phase relaxation time is
inversely proportional to the product of the mean droplet radius and droplet concentration. With
the same mean droplet radius, changes in the concentration explain the factor of about five shifts
between SDS.650, SDS.130, and SDS.26 for the low TKE case as shown in the left panel and in
Table 2. However, for the high TKE, the scaling breaks down because the phase relaxation time
485   is no longer much smaller than the turbulence integral time scale. For a given droplet
concentration, shift from low to high TKE should result to ten-fold increase of σ_S because of the
$<w^2>^{1/2}$ increase. This is approximately valid for 650 cm^{-3} droplet concentration, but reduces to a
factor of only about 5 for 26 cm^{-3} concentration.

490   The supersaturation standard deviation shown in Fig. 4 can be compared to the standard
deviation resulting from the quasi-equilibrium supersaturation fluctuations. Evolution of the
supersaturation $S = q_v/q_{vs}$ -1 (where q_{vs} is the saturated water vapor mixing ratio) can be derived
by combining Eqs. 7, 8 and 9 as

495    $\mathrm{d}S/\mathrm{d}t = a_1 w - S/\tau_{relax}$,   (10)

where τ_{relax} is the phase relaxation time that depends of the mean droplet radius and
concentration:

500    $1/\tau_{relax} = 4 \pi \rho_w A [1/q_{vs} + q_v L_v^2/(q_{vs} R_v T^2 c_p)] <N r^2/(r+r_0)>$,   (11)

where $\rho_w = 10^3$ kg m^{-3} is the water density, $R_v = 461$ J kg^{-1} K^{-1} is the water vapor gas constant, and <.> in (11) depicts averaging over all droplets within a given grid volume. The quasi-equilibrium supersaturation is obtained by setting the left-hand-side of (10) to zero that leads to

505   $S_{eq} = a_1 w \, \tau_{relax}$. For the mean temperature and humidity of the simulations and specific numerical values of the relevant constants, $a_1 = 6.54$ x 10^{-4} m^{-4} and the phase relaxation time for the 13 μm droplets and their concentration of 130 cm^{-3} is $\tau_{relax} = 1.98$ sec. The phase relaxation time is five times smaller/larger for the droplet concentration of 650/26 cm^{-3}. Since the quasi-equilibrium supersaturation is proportional to the vertical velocity, its standard deviation is

510   proportional to the rms vertical velocity. For the low TKE, the quasi-equilibrium supersaturation standard deviation is 0.120, 2.39e-2, 4.79e-3% for 26, 130 and 650 cm^{-3} droplet concentrations. These are in a relatively good agreement with simulated standard deviation shown in Table 2. The values for the high TKE should be 10 times smaller and they are approximately equal to the simulated values for 130 and 650 cm^{-3}. The agreement between the simulated supersaturation

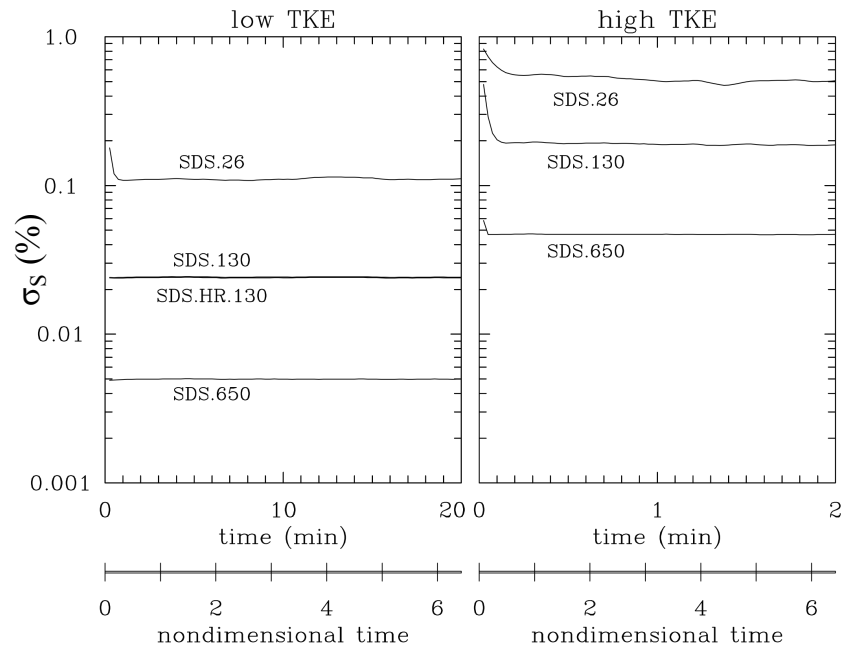
515   fluctuations and the fluctuations predicted by the quasi-equilibrium supersaturation for the 64^3 m^3 domain and low TKE agrees with results presented in Thomas et al. (2020; see Fig. 10 therein and its discussion).

520

Figure 4. Evolution of the supersaturation standard deviation in (left panel) 4 low TKE simulations and (right panel) 3 high TKE simulations with superdroplets. The two simulations with droplet concentration of 130 per cc in the left panel, SDS.130 and SDS.HR.130, show differences within the thickness of the line.

525

Figure 5 shows the comparison between the local supersaturation simulated by the model and the quasi-equilibrium supersaturation calculated applying the local vertical velocity and the mean phase relaxation time for the low and high TKE simulations and 26 versus 650 cm^{-3} droplet concentrations. The mean phase relaxation time is about 10 sec for 26 cm^{-3} and about 0.4 sec 650

530 cm^{-3} droplet concentrations. Whether the quasi-equilibrium supersaturation is a good approximation of the local supersaturation depends on the relative magnitude of the phase relaxation time scale and the eddy turnover time associated with the largest eddies. This is because the largest eddies feature the largest vertical velocities and provide the strongest forcing to drive the supersaturation away from its quasi-equilibrium value. For the low TKE, the eddy

535 turnover time associated for the largest eddies is about 1 minute (i.e., velocities up to 0.8 m s^{-1} and the domain size of 64 m), much larger than the phase relaxation time for both concentrations shown in Fig. 5. This is why all points scatter around 1:1 line in the left panels. However, the eddy turnover time is only around 8 sec for the high TKE case. This is still much larger than the phase relaxation time for the 650 cm^{-3} droplet concentration (lower right panel), but close to the

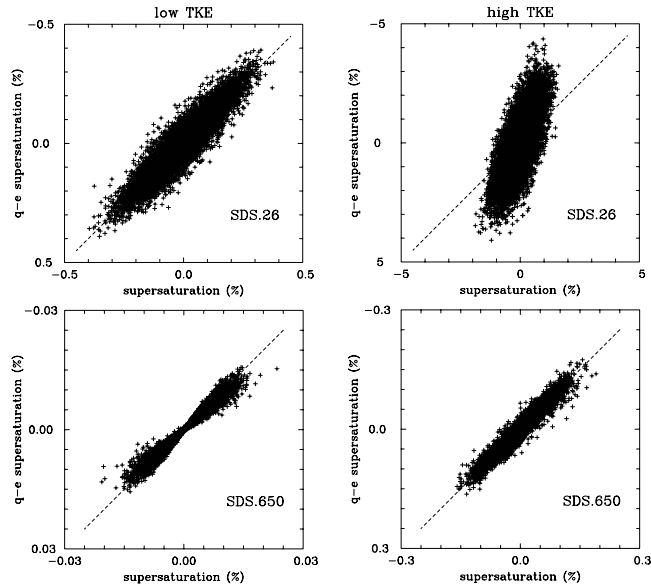
540 phase relaxation time for the 26 cm^{-3} concentration. This is why data points are scattered away from the 1:1 line in the upper right panel, with the quasi-equilibrium values typically larger (in the absolute sense) than the model-predicted supersaturation.

545

Figure 5. Comparison between supersaturation simulated by the model (horizontal axes) and the quasi-equilibrium supersaturation calculated with the local vertical velocity and the mean phase relaxation time (vertical axes) for (left panels) low TKE and (right panels) high TKE simulations. Simulations SDS.650/SDS.26 are in the lower/upper panels. Data from the last time level of all simulations with only 5% of data points shown. Note different supersaturation ranges

550   in all panels.

Figure 6 shows evolutions of the radius squared standard deviation. Sardina et al. (2015) show that the standard deviation of the radius squared distribution should increase in time as square root of time as long as the phase relaxation time is much smaller than the turbulence integral

555   time. The rate of increase is proportional to the supersaturation standard deviation (see Eq. 13 therein). The former has been shown in other numerical simulations, such as in Li et al. (2019) and Thomas et al. (2020). Fig. 6 shows that the Lagrangian microphysics reproduces the $t^{1/2}$ scaling and that the differences between various simulations for the low TKE can be explained by the differences in the supersaturation standard deviation shown in Fig. 4 (note that on the log-

560   log plot the rate of increase change corresponds to a vertical shift as shown in Fig. 6). For the high TKE, small deviations for the expected scaling can be explained by the phase relaxation time being no longer much smaller than the turbulence integral time. This is especially evident for the high-TKE SDS.26 case in the right panel of Fig. 6. Left panels of Figs. 4 and 6 show that increasing the number of superdroplets from 40 to 150 per grid volume has virtually no impact

565   on the results. Overall, the Lagrangian microphysics seems to represent expected scalings (or departures from them) without much difficulty.

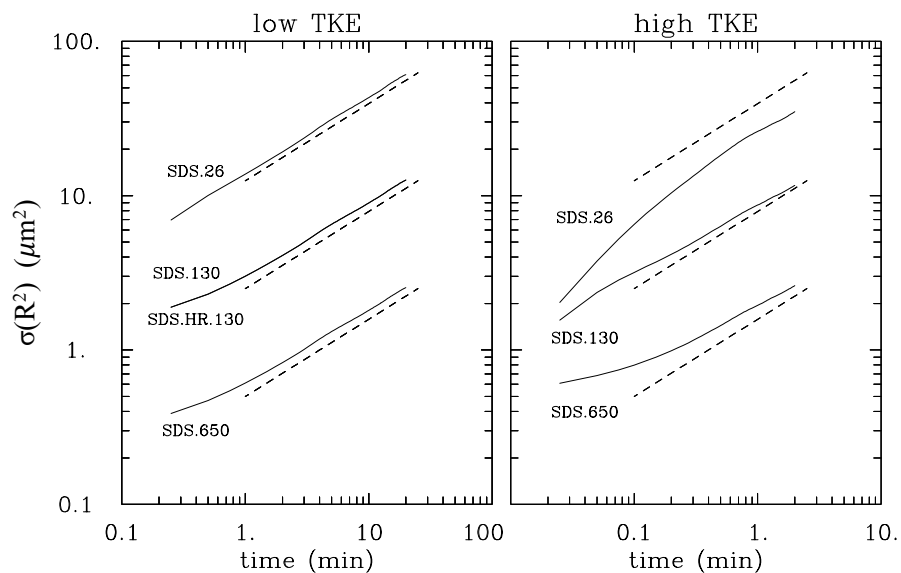



Figure 6. Evolution of the radius squared standard deviation for superdroplet simulations (left panel) 4 low TKE simulations and (right panel) 3 high TKE simulations with superdroplets. SDS.130 and SDS.HR.130 in the left panel differ by the thickness of the line. Dashed lines show expected $t^{1/2}$ scaling and are spaced by the expected factor of 5. Their position is the same in left and right panels.

Table 2. Supersaturation standard deviation (%) averaged over the last 3 integral time scales for Lagrangian microphysics simulations.

	N=26	N=130	N=650
Low TKE	0.111	2.42×10^{-2}	4.98×10^{-3}
High TKE	0.500	0.188	4.68×10^{-2}

5.2 Eulerian bin microphysics

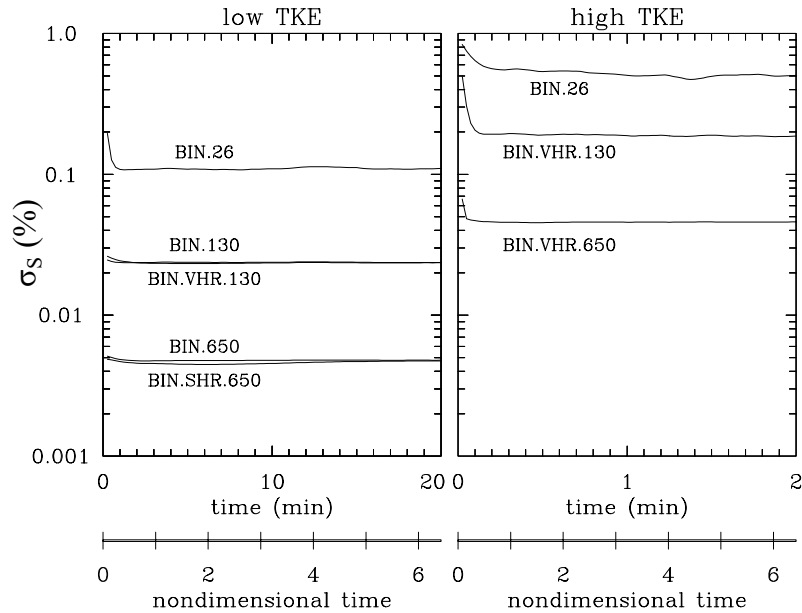



Figure 7. As Fig. 4 but for the supersaturation standard deviation in 8 simulations with bin microphysics.

590   Figures 7 and 8 show the same results as Figs. 4 and 6 for the bin microphysics. For the
        supersaturation fluctuations (Fig. 7), bin simulations match Lagrangian microphysics results, and
        the impact of bin resolution is small, at least for the low TKE simulations which feature various
        bin resolutions. However, as shown in Fig. 8, the expected $t^{1/2}$ scaling requires appropriately high
        bin resolution, and the resolution requirement changes depending of the droplet concentration.

595   The standard bin resolution is sufficient for the BIN.26 simulation. However, 130 cm^{-3}
        simulations require VHR setup (bin width of 0.1 μm) to match the expected scaling. Even the
        SHR setup (bin width of 0.05 μm) is insufficient for the 650 cm^{-3} droplet concentration. There
        are some similarities between Lagrangian and Eulerian results for the high-TKE simulations, that
        is, when the scalings derived by Sardina et al. (2015) may not apply. The left panel also shows

600   the decrease of the initial radius squared standard deviation with the increase of the bin
        resolution. This comes from the ill-posedness of the initially monodisperse droplet size
        distribution for the bin microphysics. The comparison between the local supersaturation
        predicted by the model and the quasi-equilibrium supersaturation calculated using the local
        vertical velocity (i.e., Fig. 5) for the bin microphysics is similar to that shown for the Lagrangian

605   scheme and is not shown.

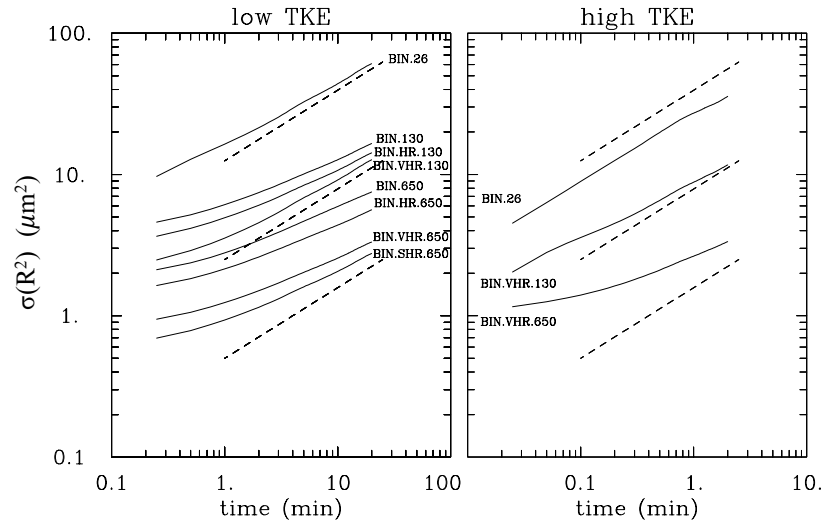



Figure 8. Evolution of the radius squared standard deviation for bin simulations. Dashed lines show the expected t[1/2] scaling. Their positions are exactly as in Fig. 6 for the Lagrangian microphysics.

In summary, Eulerian bin microphysics is capable in appropriately representing turbulent temperature and moisture fluctuations, but fails to simulate their impact on droplet spectra unless appropriately high bin resolution is used. This is further supported by the comparison of droplet spectra discussed in the next section.

5.3 Comparison of radius squared distributions between Eulerian and Lagrangian simulations.

This section compares radius squared (R^2) distributions at the end of the simulations, that is, after 6 turnover times, for both the low and high TKE simulations. As shown in Lanotte et al. (2009) and Sardina et al. (2015), an initial monodisperse distribution should evolve into a Gaussian R^2 spectrum because of the parabolic cloud droplet growth equation. Although the parabolic growth is only approximately valid because of the specific droplet growth equation (see Eq. 9), the Gaussian distribution is a good fit for simulation results discussed here as shown below.

Figure 9 shows the spectra for selected superdroplet simulations. The radius squared spectra are created by selecting R^2 bin size and binning superdroplet radii for a given simulation into the assumed bin grid. The bin size for the SDS.650/SDS.26 simulations (lower/upper panels in Fig.9) is $1/10$ μm^2. There are two panels for each simulation, one with the linear vertical scale

and the spectrum shown as a histogram, and the second one with the logarithmic vertical scale and using star symbols to show the spectrum. In addition, the logarithmic plots show the Gaussian distributions obtained with the mean and standard deviation calculated from the spectra.

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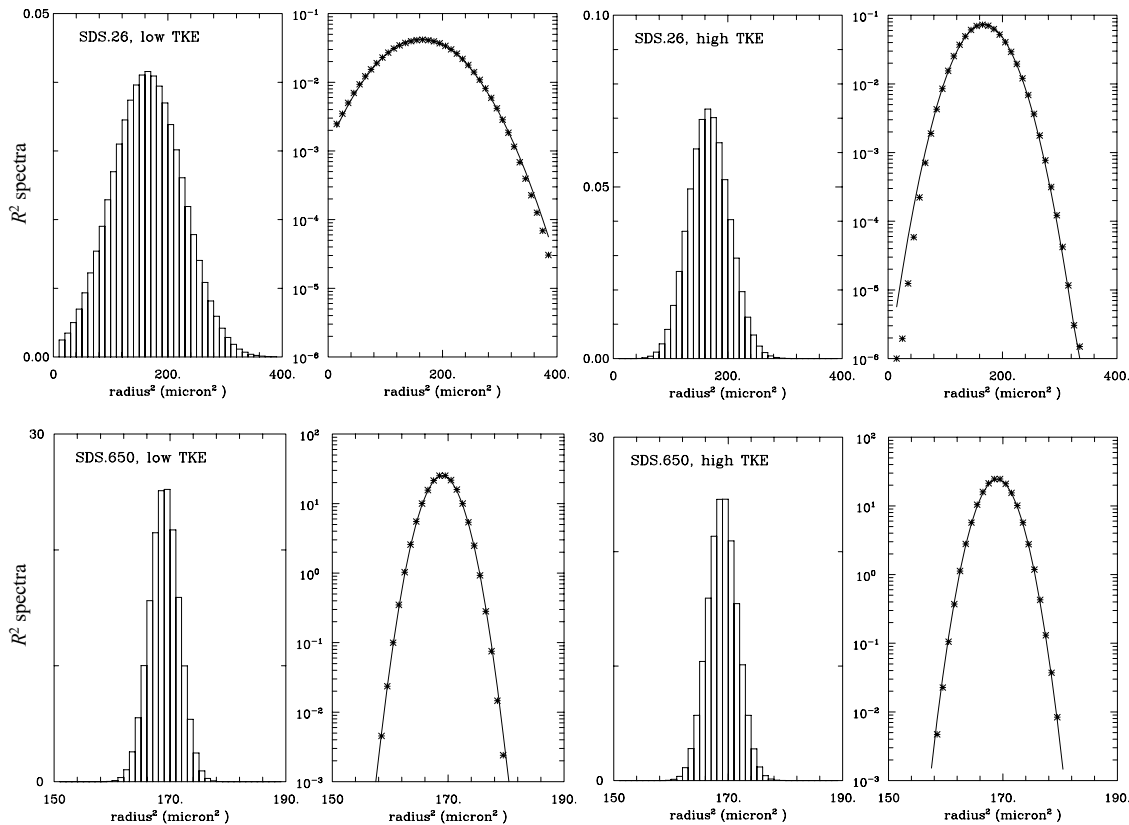


Figure 9. Results from simulations (upper panels) SDS.26 and (lower panels) SDS.650 superdroplet simulations. There
640 **are two panels for each simulation, the left one applying the linear vertical scale and the right one applying the logarithmic scale. The line in the logarithmic scale panels shows the Gaussian distribution with the mean and standard deviation calculated from the spectrum. Left/right pair in each row is for low/high TKE simulation.**

For the SDS.650 simulations (lower panels in Fig. 9), the spectra at the end of low and high TKE
645 simulations are practically the same. This agrees with the theoretical scaling and simulation results shown in Fig. 4 and 6. In contrast, results for SDS.26 differ drastically between the low and high TKE. The spectrum for the low TKE is wide, with some small droplets already evaporated because the spectrum is truncated at the low-radius end. Nevertheless, the Gaussian shape is still a good fit for the simulated spectrum. The high TKE SDS.26 spectrum is
650 significantly narrower with small deviations from the Gaussian fit.

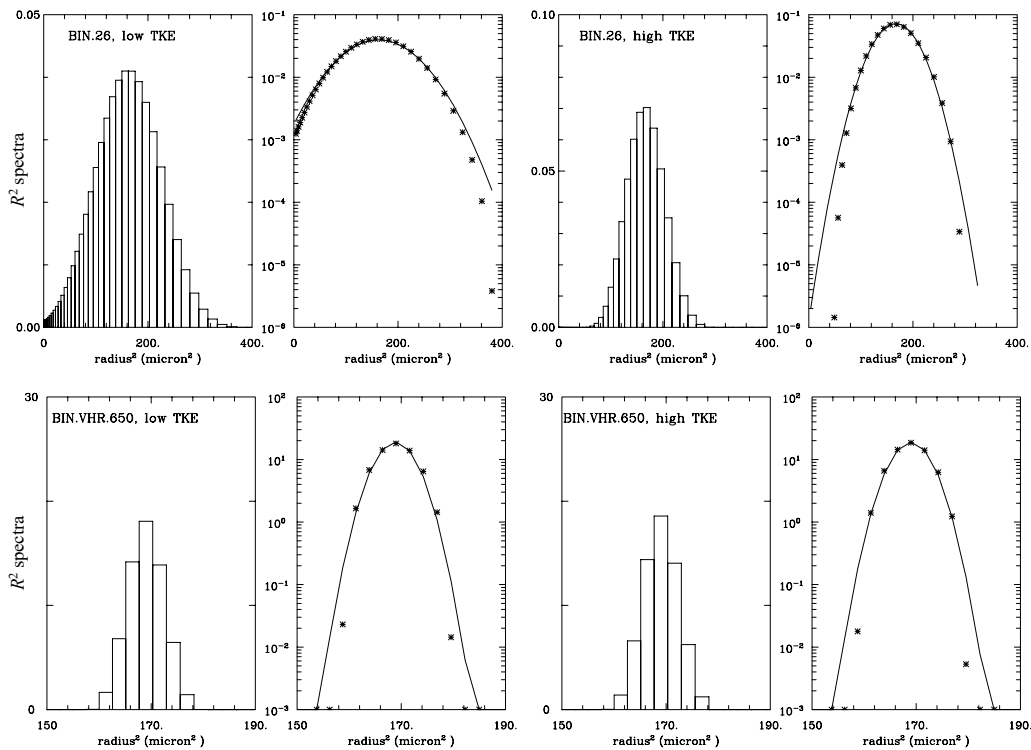



Figure 10. As Fig. 9, but for the bin (upper panels) BIN.26 and (lower panels) BIN.VHR.650 simulations.

Figure 10 shows the spectra for bin simulations similar to those in Fig. 9. Since bin simulations predict the spectra directly, the radius spectra are converted to R^2 spectra and then plotted at their native resolution in the R^2 space. This explains the change in the resolution along the horizontal axes evident in the upper panels. Overall, there are some similarities between Figs. 9 and 10. For instance, upper panels show spectra for the 26 cm^{-3} simulations with 0.5-μm bin width that are similar to those in superdroplet simulations. Spectra for 650 cm^{-3} simulations with 0.1-μm bin width (i.e., from the VHR set) are also similar between low and high TKE simulations, but their spectral widths are larger than in corresponding panels of Fig. 9. The impact of the bin resolution is further documented in Fig. 11 that shows results from the 650 cm^{-3} low TKE HR and SHR simulations, that is, with the bin width of 0.3 and 0.05 μm, respectively. Only the SHR simulation (i.e., the right panel in Fig. 11) resembles the spectra from the Lagrangian simulations shown in the lower panels of Fig. 9.

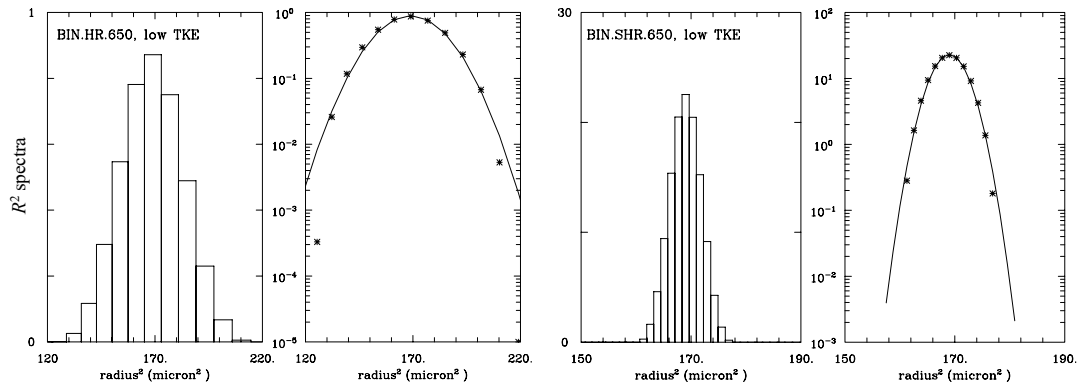



Fig. 11. As Figs. 9 and 10, but for the bin BIN.HR.650 and BIN.SHR.650 simulations. Note different horizontal range at the left and right pair of panels.

675

In summary, only extreme resolutions of the bin scheme (e.g., as in SHR, 0.05 μm bin width) allow good agreements between Lagrangian and Eulerian results for the concentration range considered here. Moreover, the ill-posed initial condition for the Eulerian scheme (i.e., the monodisperse initial droplet size distribution) seems irrelevant because the spectrum becomes

680 well-resolved after some time during the simulation. With sufficiently high bin resolution, (e.g., 0.5 μm in the 26 cm^{-3} simulations or 0.05 μm for the 650 cm^{-3} simulations), the Eulerian and Lagrangian spectra compare well at the end of the simulations. This shows the benefit of the Lagrangian scheme as one does not have to worry about the bin size to obtain numerically converged solutions.

685

6 Grid volume by grid volume analysis of macro- and microphysical properties

The analysis presented in previous sections concerns domain-averaged characteristics. Because all simulations with either low or high TKE feature exactly the same evolving flow field,

690 simulated thermodynamic variables (i.e., the temperature, water vapor, and cloud droplet characteristics) can be compared grid volume by grid volume and thus provide a comprehensive comparison of simulated local conditions. Such a comparison is in the spirit of the piggybacking methodology applied in G20b.

695 Figure 12 compares the temperature, water vapor, and cloud water mixing ratios (the latter derived from the predicted droplet spectra within each grid volume) between SDS.130 and BIN.130 low TKE simulations at time of 20 minutes. For the temperature and moisture, plots at

earlier times are similar to upper panels in Fig. 12 except for smaller ranges between minima and maxima. Cloud water plots at earlier times are also similar to those shown in Fig. 12 except for

700   the initial couple minutes. The temperature and water vapor values are extremely close between the two simulations: the root mean square difference between temperatures are 2.6×10^{-4} K. For the water vapor mixing ratios, the root mean square difference is 1.1×10^{-4} g kg^{-1}. However, the cloud water mixing ratio can differ significantly between the bin and the superdroplet simulations. This is because of statistical fluctuations in the number of superdroplets per grid

705   volume. With on average 40 superdroplets per grid volume, the standard deviation of the droplet number is around 6, or about 15% of the mean. Assuming that one can find grid volumes with three times the standard deviation, the range of the cloud water mixing ratio can be as high as close to 50%. This can explain the spread seen in the lower left panel of Fig. 12. With 150 superdroplets per grid volume in SDS.HR.130, there is some improvement as the standard

710   deviation is reduced to about 8% of the mean, but the statistical fluctuations remain significant. In fact, the lower left panel does not change significantly if SDS.130 is replaced by SDS.HR.130 (not shown). The lower right panel shows the outcome of a simple rescaling of the cloud water mixing ratio q_c predicted by the Lagrangian scheme based on the number of superdroplets N being present in a given grid volume compared to the expected mean value of 40, with the

715   rescaled cloud water mixing ratio given by q_c $40/N$ (i.e., increased when $N < 40$ and reduced when $N > 40$). We stress that the rescaling is done on the analyzed cloud water, and not during the model run. (That said, application of such a rescaling might be a valuable approach to reduce the spread during model run as well; this aspect is left for a future investigation). Apparently, the rescaling improves the comparison significantly and documents that the scatter present in the

720   lower left panel comes predominantly from the statistical fluctuations in the Lagrangian scheme. An important point is that the cloud water fluctuations are short-lived. This is because the temperature and water vapor would feature larger scatter if the fluctuations in the grid volume superdroplet number were long-lived. These statistical fluctuations come only from superdroplet advection by the resolved flow as the inertial effects and droplet sedimentation are not

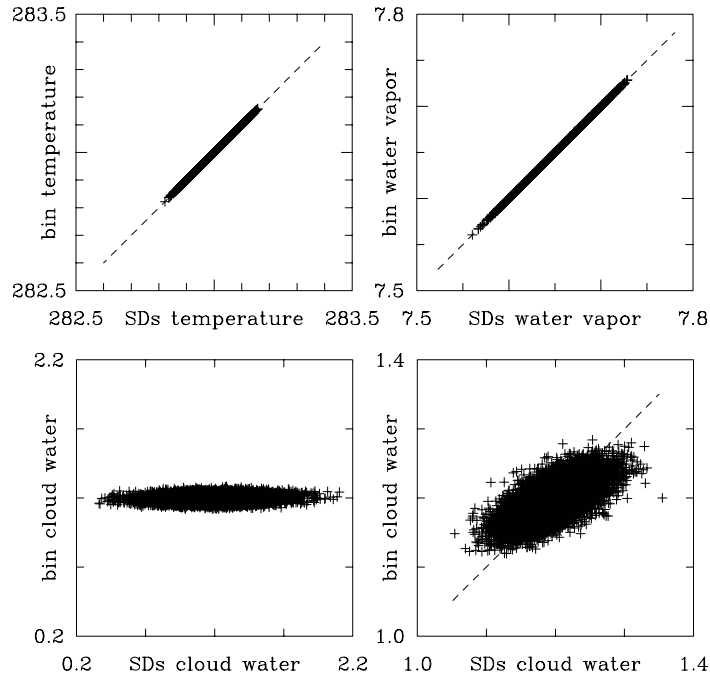
725   considered.

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Figure 12. Grid volume by grid volume comparison for the low TKE SDS.130 and BIN.130 simulations between (upper left) temperature (in K), (upper right) water vapor mixing ratio (in g kg⁻¹), and (lower left) cloud water mixing ratio (in g kg⁻¹) at minute 20. The lower right panel shows cloud water mixing ratio comparison after the SDS.130 results are adjusted as explained in the text. Note the change of horizontal and vertical scales between lower left and lower right

735 **panels. Only 5% of data points are used.**

Figure 13, in the format of Fig. 12, compares the grid volume mean radii and spectral width in two sets of low-TKE simulations, the standard resolution (SDS.130 and BIN.130) and the increased resolution (SDS.HR.130 and BIN.VHR.130). For the increased bin resolution, the

740 selected bin microphysics is the one that shows the correct scaling in Fig. 8. The mean radius comparison features some scatter that is reduced when increased resolutions simulations are compared. However, the scatter is asymmetric with respect to 1:1 line and similar to the cloud water scatter in the lower right panel of Fig. 12. The asymmetry shows that the bin microphysics tends to simulate larger droplets than the Lagrangian microphysics for droplets smaller than the

745 mean, and the reverse is true for droplets larger than the mean. The spectral width panels show that the bin simulations feature smaller spread of the spectral width across the computational domain than the Lagrangian scheme. This seems independent of the bin resolution. In other words, spectral width simulated by the bin scheme varies less across the computational domain. In contrast, superdroplet simulations feature larger spread of the spectral width across the

750 domain, and the spread decreases with the increase of the mean superdroplet number per grid

volume. For the SDS.130 versus BIN.130 cloud of spectral width points (i.e., the upper right

panel), the center of mass is above the 1:1 line. This implies that the mean spectral width for

BIN.130 simulation is overpredicted, in agreement with the results shown in Fig. 8. Results for

similar comparisons of other simulations (for instance, SDS.26 versus BIN.26 or SDS.650 and

755 BIN.SHR.650) are similar except for different ranges of the mean radius and spectral width (not

shown). As shown in Fig. 14, the high TKE simulations also show similar patterns, with changes

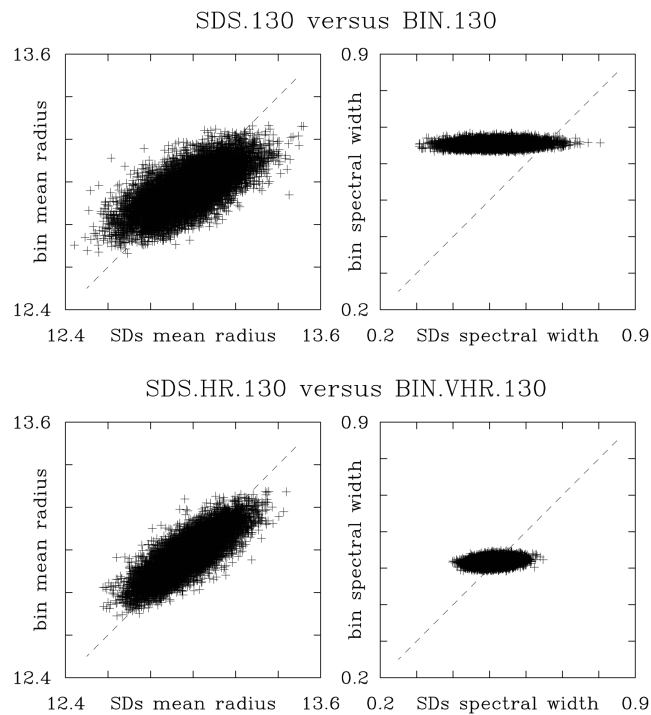
consistent with the differences in right panels in Figs. 6 and 8.

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Figure 13. Grid volume by grid volume comparison at the end of low TKE simulations (20 min) between (left panels) the grid-volume mean radius (in microns) and (right panels) spectral width (in microns). Lower (upper) panels are for comparison between SDS.HR.130 and BIN.VHR.130 (SDS.130 and BIN.130). Only 5% of data points are used.

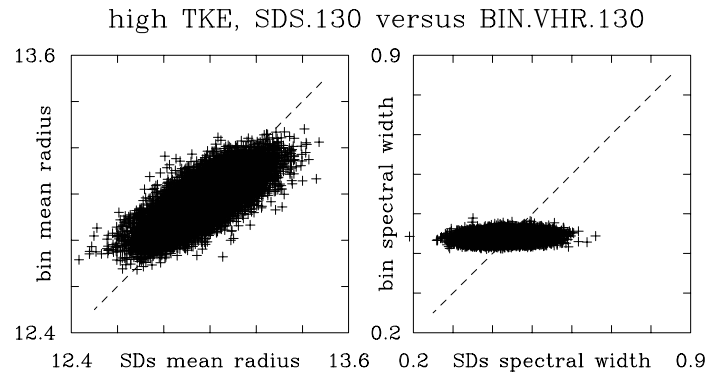
765

In summary, the grid volume by grid volume comparison between Eulerian and Lagrangian

results shows that the simulated spatial variability is smaller in the bin microphysics when

compared to the superdroplets. Arguably, this comes from a combination of the numerical

diffusion in the bin microphysics (i.e., smoothing bin results similar to other Eulerian fields) and

770   small-scale fluctuations of the Lagrangian microphysics due to a relatively small mean number
of superdroplets per grid volume.

775   **Figure 14. As Fig. 10, but for SDS.130 and BIN.VHR.130 simulations with high TKE.**

7 Summary and conclusions

This paper presents a modeling study addressing the impact of homogeneous isotropic turbulence
780   on the broadening of initially monodisperse distribution of cloud droplets in response to local
fluctuations of the supersaturation field. This problem has been considered previously in
modeling studies of Lanotte et al. (2009) applying DNS, Thomas et al. (2020) using the scaled-
up DNS, and Sardina et al. (2015) employing theoretical analysis combined with DNS and
stochastic model simulations. Sardina et al. (2015) derived scaling relationships that we use in
785   validating model results and comparing results for different droplet concentrations and
contrasting turbulence intensities.

Because we apply a finite-difference fluid flow model, we had to develop a turbulence forcing
scheme that led to the quasi-steady homogeneous isotropic turbulence similar to that simulated
790   by a spectral model. The forcing scheme applied here is in the spirit of the linear forcing of
Rosales and Meneveau (2005) and Onishi et al. (2011). The idea is to ensure that the mean
turbulence kinetic energy (TKE) remains constant in time and that the partitioning between the
three TKE components does not change. The latter is important for the simulations of the
turbulence impact on the droplet spectra because the driving mechanism in the homogeneous

795 environment comes from the vertical velocity fluctuations affecting the local supersaturation. The simulations are in the spirit of the implicit large eddy simulation (ILES), that is, without modeling the small-scale TKE and scalar variance dissipation (Margolin and Rider, 2002; Andrejczuk et al., 2004; Margolin et al., 2006; Grinstein et al., 2007). ILES applying a finite difference model relies on the model numerics to provide the required dissipation, in contrast to

800 the scaled-up spectral model DNS in Thomas et al. (2020) where appropriately scaled-up molecular dissipation coefficients have to be used to ensure stable simulations. The TKE dissipation rate diagnosed from the forcing algorithm (see Eq. 6) is approximately correct for the considered turbulence intensities.

805 There are two drastically different simulation techniques that can be applied to investigate the impact of cloud turbulence on the droplet spectra: the Eulerian bin microphysics and the Lagrangian particle-based approach, the latter often referred to as the superdroplet method (see review in the introduction). We apply the ILES homogeneous isotropic turbulence setup to compare the two techniques following Li et al. (2017), Grabowski (2020a), and Grabowski

810 (2020b) for the diffusional growth of cloud droplets only. The computational domain is 64^3 m^3, one of the domain sizes considered in Thomas et al. (2020) and similar to grid volumes of a typical LES simulation of natural clouds. Two TKE intensities are considered, low and high, different by a factor of one hundred. The latter implies that the velocity fluctuation differ by a factor of ten and the TKE dissipation rates differ by a factor of one thousand. The TKE

815 dissipation spans the range observed in natural clouds.

The Lagrangian approach reproduces the expected scalings derived in Sardina et al. (2015) for the case when the turbulence integral time scale is much longer that the phase relaxation time of cloud droplets. Representing the scalings is more challenging for the bin microphysics because

820 appropriately high resolution in the bin space is needed. In fact, the standard bin resolution, with the bin width of 0.5 μm and covering the range up to 20 μm, similar to Grabowski (2020a, 2020b), is only sufficient for the lowest droplet concentration (26 cm^{-3}). For the highest droplet concentration, 650 cm^{-3}, even an order of magnitude smaller bin size is not sufficient to reproduce well the expected scaling. Such a bin resolution is impossible to use when collisional

825 growth is also considered as in Li et al. (2017). For the lowest droplet concentration (26 cm^{-3})

and the high TKE case, the phase relaxation time is about 10 sec and the turbulence integral time is around 19 sec, so some departures from the expected scaling are expected. This is indeed the case, and the two simulation methodologies represent similar supersaturation and spectral width departures.

830

Because the fluid flow is the same for all simulations featuring either low or high TKE, one can compare model results point-by-point as in the piggybacking technique of Grabowski (2019). Such a comparison shows miniscule differences between temperature and water vapor fields across the computational domain, and larger differences between simulated mean droplet radii and spectral width. These are consistent with fundamental differences in the two simulation methodologies, numerical diffusion in the Eulerian approach and relatively small number of Lagrangian particles (superdroplets) that can be afforded in the particle-based microphysics. Either one can be limited by either increasing the model resolution or increasing the number of Lagrangian particles, both significantly increasing computational cost. But there are additional options for the particle-based microphysics, for instance, assuming that a particle within a given grid volume represents a cloud of particles spread over a prescribed halo. We are pursuing those ideas in ongoing research.

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Data availability. Data supporting this study is available at
845   https://dashrepo.ucar.edu/dataset/144_grabow.html, (https://doi.org/10.5065/2ybq-nd09). Last accessed 14 January 2021.

Author contributions. WWG developed the idea and ran the simulations. WWG and LT performed data analysis and prepared the manuscript.

850

Competing interests. The authors declare that they have no conflict of interest.

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855   from-home period due to the COVID-19 pandemic. Initial flow data that were used to initiate the simulations were provided by JPL's Dr. Marcin Kurowski. WWG acknowledges partial support

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References

Andrejczuk, M., Grabowski, W. W., Malinowski, S. P., and Smolarkiewicz P. K.: Numerical
865   simulation of cloud– clear air interfacial mixing, J. Atmos. Sci., 61, 1726–1739, 2004.

Andrejczuk, M., Reisner, J. M., Henson, B., Dubey, M. K., and Jeffery, C. A.: The potential impacts of pollution on a nondrizzling stratus deck: Does aerosol number matter more than type?, J. Geophys. Res., 113, D19204, doi:10.1029/ 2007JD009445, 2008.
870

Arabas, S., Jaruga, A., Pawlowska, H., and Grabowski, W. W.: libcloudph++ 1.0: a single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++, Geosci. Model Dev., 8, 1677–1707, https://doi.org/10.5194/gmd-8-1677- 2015, 2015.

875   Arabas, S. and Shima, S.-I.: Large-eddy simulations of trade wind cumuli using particle-based microphysics with Monte Carlo coalescence, J. Atmos. Sci., 70, 2768-2777, https:// doi.org/10.1175/JAS-D-12-0295.1, 2013.

Benmoshe, N., Pinsky, M., Pokrovsky, A., and Khain, A.: Turbulent effects on the microphysics
880   and initiation of warm rain in deep convective clouds: 2-D simulations by a spectral mixed-phase microphysics cloud model, J. Geophys. Res., 117, D06220, doi:10.1029/2011JD016603, 2012.

Clark, T. L.: Numerical modeling of the dynamics and microphysics of warm cumulus convection, J. Atmos. Sci., 30, 857-878, 1973.
885

Dziekan, P., Waruszewski, M., and Pawlowska, H.: University of Warsaw Lagrangian cloud model (UWLCM) 1.0: A modern large-eddy simulation tool for warm cloud modeling with

Lagrangian microphysics, Geosci. Model Dev., 12(6), 2587–2606, doi: 10.5194/gmd-12-2587-2019, 2019.

890

Grabowski, W. W. (G20a): Comparison of Eulerian bin and Lagrangian particle-based schemes in simulations of Pi Chamber dynamics and microphysics, J. Atmos. Sci., 77, 1151-1165, 2020.

Grabowski, W. W. (G20b): Comparison of Eulerian bin and Lagrangian particle-based

895 microphysics in simulations of nonprecipitating cumulus, J. Atmos. Sci., 77, 3951-3970, 2020.

Grabowski, W. W.: Separating physical impacts from natural variability using piggybacking technique, Adv. Geosci., 49, 105-111, 2019.

900 Grabowski, W. W. and Abade, G. C.: Broadening of cloud droplet spectra through eddy hopping: Turbulent adiabatic parcel simulations, J. Atmos. Sci., 74, 1485-1493, 2017.

Grabowski, W. W., Andrejczuk, M., and Wang, L.-P.: Droplet growth in a bin warm-rain scheme with Twomey CCN activation, Atmos. Res., 99, 290–301, 2011.

905

Grabowski, W. W., Dziekan, P., and Pawlowska, H.: Lagrangian condensation microphysics with Twomey CCN activation. Geosci. Model Dev., 11, 103-120, 2018.

Grabowski, W. W., Morrison, H., Shima, S.-I., Abade, G. C., Dziekan, P., and Pawlowska, H.:

910 Modeling of cloud microphysics: Can we do better? Bull. Amer. Meteor. Soc., 100, 655-672, https:// doi.org/10.1175/BAMS-D-18-0005.1, 2019.

Grinstein, F. F., Margolin, L. G., and Rider, W. J.: Implicit Large Eddy Simulation: Computing Turbulent Fluid Dynamics, Cambridge University Press, 2007.

915

Hoffmann, F., Yamaguchi, T., and Feingold, G.: Inhomogeneous mixing in Lagrangian cloud models: Effects on the production of precipitation embryos, J. Atmos. Sci., 76, 113–133, https:// doi.org/10.1175/JAS-D-18-0087.1, 2019.

920   Khain, A. P., and Coauthors.: Representation of microphysical processes in cloud-resolving models: Spectral (bin) microphysics versus bulk parameterization, Rev. Geophys., 53, 247-322, https://doi.org/10.1002/2014RG000468, 2015.

Kogan, Y. L.: The simulation of a convective cloud in a 3-D model with explicit microphysics.
925   Part I: Model description and sensitivity experiments. J. Atmos. Sci., 48, 1160–1189, https://doi.org/10.1175/1520-0469(1991)048,1160:TSOACC. 2.0.CO;2, 1991.

Lanotte, A. S., Seminara, A., and Toschi, F.: Cloud droplet growth by condensation in homogeneous isotropic turbulence, J. Atmos. Sci., 66, 1685–1697, 2009.
930

Lasher-Trapp, S. G., Cooper, W. A., and Blyth, A. M.: Broadening of droplet size distributions from entrainment and mixing in a cumulus cloud, Quart. J. Roy. Meteor. Soc., 131, 195-220, https://doi.org/10.1256/q j.03.199, 2005.

935   Li, X.-Y., Brandenburg, A., Haugen, N. E. L., and Svensson, G.: Eulerian and Lagrangian approaches to multidimensional condensation and collection, J. Adv. Model. Earth Syst., 9, 1116–1137, doi:10.1002/2017MS000930, 2017.

Li, X.-Y., Svensson, G., Brandenburg, A., and Haugen, N. E. L.: Cloud-droplet growth due to
940   supersaturation fluctuations in stratiform clouds, Atmos. Chem. Phys., 19, 639–648, https://doi.org/10.5194/acp-19-639-2019, 2019.

Margolin, L. G., Rider, W. J., and Grinstein, F. F.: Modeling turbulent flow with implicit les, J. Turbul., 7, N15, doi:10.1080/ 14685240500331595, 2006.
945

Margolin, L. G., and Rider, W. J.: A rationale for implicit turbulence modelling, Int. J. Numer. Methods Fluids., 39, 821-841, 2002.

Mordy, W.: Computations of the growth by condensation of a population of cloud droplets.
Tellus, 11: 16-44. https://doi.org/10.1111/j.2153-3490.1959.tb00003.x, 1959.

Morrison, H., Witte, M., Bryan, G. H., Harrington, J. Y., and Lebo, Z. J.: Broadening of modeled cloud droplet spectra using bin microphysics in an Eulerian spatial domain. J. Atmos. Sci., 75, 4005-4030, https://doi.org/10.1175/JAS-D-18-0055.1, 2018.

Onishi, R., Baba, Y., and Takahashi, K.: Large-scale forcing with less communication in finite-difference simulations of stationary isotropic turbulence, J. Comp. Phys., 230, 4088–4099, 2011.

Riechelmann, T., Noh, Y., and Raasch, S.: A new method for large-eddy simulations of clouds with Lagrangian droplets including the effects of turbulent collision, New J. Phys., 14, 065008, https://doi .org/10.1088/1367-2630/14/6/065008, 2012.

Rosales, C., and Meneveau, C.: Linear forcing in numerical simulations of isotropic turbulence: Physical space implementations and convergence properties, Phys. Fluids., 17, 095106, 2005.

Sardina, G., Picano, F., Brandt, L., and Caballero, R.: Continuous growth of droplet size variance due to condensation in turbulent clouds, Phys. Rev. Lett., 115, 184501, https://doi.org/10.1103/PhysRevLett.115.184501, 2015.

Shima, S.-I., Kusano, K., Kawano, A., Sugiyama, T., and Kawahara, S.: The superdroplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model, Quart. J. Roy. Meteor. Soc., 135, 1307-1320, https://doi.org/10.1002 /qj.441, 2009.

Siebert, H., Lehmann, K., and Wendisch, M.: Observations of small-Scale turbulence and energy dissipation rates in the cloudy boundary layer, J. Atmos. Sci., 63, 1451–1466, 2006.

Siebesma, A. P., and Coauthors.: A large eddy simulation intercomparison study of shallow cumulus convection, J. Atmos. Sci., 60, 1201–1219, doi:10.1175/1520-0469(2003)60,1201: ALESIS.2.0.CO;2, 2003.

980

Stevens, B., and Coauthors.: Evaluation of large-eddy simulations via observations of nocturnal marine stratocumulus, Mon. Wea. Rev., 133, 1443–1462, 2005.

985 Thomas, L., Grabowski, W. W., and Kumar, B.: Diffusional growth of cloud droplets in homogeneous isotropic turbulence: DNS, scaled-up DNS, and stochastic model, Atmos. Chem. Phys., 20, 9087-9100, 2020.

Unterstrasser, S., Hoffmann, F., and Lerch, M.: Collection/aggregation algorithms in Lagrangian

990 cloud microphysical models: Rigorous evaluation in box model simulations, Geosci. Model Dev., 10, 1521–1548, https://doi .org/10.5194/gmd-10-1521-2017, 2017.

Vaillancourt, P., Yau, M. K., and Grabowski, W. W.: Microscopic approach to cloud droplet growth by condensation. Part I: Model description and results without turbulence, J. Atmos. Sci.,

995 58, 1945–1964, 2001.

Vaillancourt, P. A., Yau, M. K., Bartello, P., and Grabowski, W. W.: Microscopic approach to cloud droplet growth by condensation. Part II: Turbulence, clustering and condensational growth, J. Atmos. Sci., 59, 3421–3435, 2002.

1000

VanZanten, M. C. and Coauthors.: Controls on precipitation and cloudiness in simulations of trade-wind cumulus as observed during RICO, J. Adv. Model. Earth Syst., 3, M06001, https://doi.org/10.1029/2011MS000056, 2011.

1005