Homogeneity of the Subgrid-Scale Turbulent Mixing in Large-Eddy Simulation of Shallow Convection

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ABSTRACT

This paper presents an approach to locally predict homogeneity of the subgrid-scale turbulent mixing in large-eddy simulation of shallow clouds applying double-moment warm-rain microphysics. The homogeneity of subgrid-scale mixing refers to the partitioning of the cloud water evaporation due to parameterized entrainment between changes of the mean droplet radius and changes of the mean droplet concentration. Homogeneous and extremely inhomogeneous mixing represent two limits of possible scenarios, where the droplet concentration and the mean droplet radius remains unchanged during the microphysical adjustment, respectively. To predict the subgrid-scale mixing scenario, the double-moment microphysics scheme is merged with the approach to delay droplet evaporation resulting from entrainment. Details of the new scheme and its application in the Barbados Oceanographic and Meteorological Experiment (BOMEX) shallow convection case are discussed. The simulated homogeneity of mixing varies significantly inside small convective clouds, from close to homogeneous to close to extremely inhomogeneous. The mean mixing characteristics become more homogeneous with height, reflecting increases of the mean droplet size and the mean turbulence intensity, both favoring homogeneous mixing. Model results are consistent with microphysical effects of entrainment and mixing deduced from field observations. Mixing close to homogeneous is predicted in volumes with the highest liquid water content (LWC) and strongest updraft at a given height, whereas mixing in strongly diluted volumes is typically close to extremely inhomogeneous. The simulated homogeneity of mixing has a small impact on mean microphysical characteristics. This result agrees with the previous study applying prescribed mixing scenarios and can be explained by the high humidity of the clear air involved in the subgrid-scale mixing.

1. Introduction

Large-eddy simulation (LES) models provide an indispensible tool to study processes within cloud-topped subtropical and trade wind boundary layers (e.g., Siebesma et al. 2003, Stevens et al. 2005, and references therein). The entire premise of the LES approach is that mean features of the turbulent flow are determined predominantly by the behavior of large (energy containing) scales of motion, with smaller scales (down to the dissipation scale) slaved to the large eddies. Although this might be true for dry atmospheric dynamics, it is uncertain if such reasoning is valid for clouds. Since cloud droplets grow or evaporate in response to molecular processes in their immediate vicinity, details of small-scale processes do matter. This is especially true for the entrainment and mixing between a cloud and its environment and for the impact that entrainment has on the spectrum of cloud droplets. Since shallow convective clouds are strongly diluted by entrainment [e.g., Warner

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(1955) and numerous subsequent studies (e.g., Gerber et al. 2005; Arabas et al. 2009)], interactions between small-scale cloud dynamics and microphysics are particularly relevant.

The impact of entrainment and mixing on the cloud droplet spectrum is poorly understood and it is unclear how observed features are influenced by instrumental artifacts (e.g., Burnet and Brenguier 2007; Chosson et al. 2007; Lu et al. 2011). Entrainment leads to a reduction of the liquid water content (LWC), but its effect on the droplet spectrum is poorly understood. The key issue is whether the evaporation due to mixing results in a reduction of only the droplet size (as in homogeneous mixing), both the number of droplets and their sizes (as in inhomogeneous mixing), or only the number of droplets (as in extremely inhomogeneous mixing). The homogeneity of mixing depends on the relative magnitude of the time scales for droplet evaporation and for turbulent homogenization (Baker and Latham 1979; Baker et al. 1980; Jensen and Baker 1989; Burnet and Brenguier 2007; Andrejczuk et al. 2009; Lehmann et al. 2009). The ratio of the two time scales is an analog of the Damkohler number in chemically reacting turbulent flows (Jeffery and Reisner 2006). Homogeneous mixing takes place when the turbulent homogenization time scale is much smaller than the droplet evaporation time scale because all droplets are then exposed to the same conditions during evaporation. In the opposite limit, when the turbulent homogenization time scale is much longer than the droplet evaporation time scale, extremely inhomogeneous mixing is thought to occur, with some droplets evaporating completely and the rest not experiencing any evaporation at all. Some studies argue that homogeneous mixing should dominate in convective clouds (Jensen et al. 1985; Jensen and Baker 1989), while others imply inhomogeneous mixing (Pawlowska et al. 2000). Recent studies suggest that various mixing scenarios can occur in a single cloud (Burnet and Brenguier 2007; Andrejczuk et al. 2009; Lehmann et al. 2009). Instead of considering a single scale, it is more appropriate to consider a continuum of scales during entrainment with the time scale, and thus the mixing scenario, calculated locally (Lehmann et al. 2009). Mixing scenarios may also change during cloud evolution. Burnet and Brenguier (2007) suggest that less diluted cumulus clouds may feature predominantly homogeneous mixing, but more diluted clouds (perhaps later in their life cycle) may be dominated by inhomogeneous mixing. Lehmann et al. (2009) show that actively growing young clouds tend to mix in a more homogeneous way. In clouds that are more diluted and close to dissipation, Lehmann et al. (2009) observed more inhomogeneous mixing events.

The double-moment warm-rain cloud microphysics scheme of Morrison and Grabowski (2007, 2008) predicts both the mass and number mixing ratios of cloud droplets\(^1\) (as well as drizzle/raindrops, the latter only marginally relevant for this study). The scheme allows coupling various subgrid-scale-mixing scenarios to the model microphysics. This aspect was pursued in a modeling study reported in Slawinska et al. (2012, hereafter SGPM12) based on the Barbados Oceanographic and Meteorological Experiment (BOMEX; Holland and Rasmussen 1973) model intercomparison case of Siebesma et al. (2003). However, since the double-moment scheme itself does not predict the homogeneity of the subgrid-scale mixing, SGPM12 simply contrasted simulations that assumed homogeneous and extremely inhomogeneous mixing, with the mixing scenario fixed for the duration of each simulation. This was done for either polluted or pristine aerosol conditions, with the impact of the assumed scenario relatively small regardless of aerosol characteristics. In contrast to SGPM12, the current paper presents a method that allows local prediction of the homogeneity of subgrid-scale mixing by merging the double-moment microphysics scheme with an approach to represent the effects of turbulent entrainment and mixing proposed by Grabowski (2007, hereafter G07) and further refined in Jarecka et al. (2009, hereafter JGP09). The combined scheme is used here in the BOMEX simulations and the model results are put in the context of recent cloud observations.

The next section summarizes an approach developed by G07 and JGP09 to delay LWC evaporation until subgrid-scale homogenization can be assumed. JGP09 referred to this approach as the $\lambda - \beta$ subgrid-scale scheme, where $\lambda$ is the characteristic scale (width) of cloud filaments and $\beta$ is the fraction of a grid box occupied by the cloudy air. Section 2 also describes how the $\lambda - \beta$ scheme is combined with the double-moment bulk microphysics scheme of Morrison and Grabowski (2007, 2008) to locally predict the homogeneity of mixing. Details of the model setup and model simulations are presented in section 3. Results from simulations of a shallow convective cloud field that applied the new scheme and their relationship to previous studies concerning homogeneity of the subgrid-scale mixing are discussed in sections 4 and 5. Section 6 provides a discussion of model results that concludes the paper.

\(^1\)Throughout this paper, we refer to the number mixing ratio as “concentration” and express it in units of per milligram. Note that the number mixing ratio in units of per milligram is equal to the traditional droplet concentration in units of per centimeter cubed for the air density of $1 \text{ kg m}^{-3}$.
2. Merging the double-moment warm-rain microphysics scheme with the $\lambda - \beta$ scheme

In the double-moment warm-rain microphysics scheme of Morrison and Grabowski (2007, 2008), cloud droplets are assumed to follow the gamma size distribution. The slope and the intercept parameters of the distribution are derived from the predicted cloud water mixing ratio and the droplet concentration, and the shape parameter is specified as a function of the droplet concentration [cf. (2) in Morrison and Grabowski (2007)]. Raindrops are assumed to follow the Marshall–Palmer size distribution (i.e., the gamma distribution with the shape parameter set to zero), with the slope and the intercept parameters derived from the predicted rainwater mixing ratio and the raindrop concentration. The scheme also includes prediction of the in-cloud supersaturation in place of the saturation-adjustment procedure used in some double-moment warm-rain schemes. Prediction of the in-cloud supersaturation permits fresh activation of cloud droplets at the cloud base as well as throughout the cloud depth. This is critical for maintaining approximately constant-in-height mean concentration of cloud droplets in agreement with aircraft observations (see discussion in SGPM12). To represent the activation in cases when precipitation processes are active, the scheme requires prediction of the concentration of activated cloud condensation nuclei (CCN); see Morrison and Grabowski (2008). The $\lambda - \beta$ scheme adds two predicted variables: the characteristic scale (width) of cloud filaments and the fraction of a grid box occupied by the cloudy air. The evolution equations for these variables are exactly as in JGP09 [see (2) and (4) therein]. The reader is referred to G07 and JGP09 for a detailed discussion of the $\lambda - \beta$ scheme and examples of its application in a single-moment bulk cloud model.

Combining the $\lambda - \beta$ scheme with the double-moment microphysics scheme involves two issues. The first one concerns the delay of cloud water evaporation during the turbulent stirring. It was argued in G07 and JGP09 that evaporation of cloud droplets resulting from the parameterized subgrid-scale mixing should be delayed until the grid box is homogenized at the cloud microscale; that is, $\lambda$ becomes smaller than the assumed threshold $\lambda_0$ [which should be on the order of the Kolmogorov microscale $\eta = (\nu/\epsilon)^{1/4}$, where $\nu$ is the air kinematic viscosity and $\epsilon$ is the dissipation rate of turbulent kinetic energy; $\eta \sim 1$ mm in typical atmospheric conditions]. However, in contrast to G07 and JGP09, one might anticipate a gradual increase of the evaporation when $\lambda_0$ is approached, instead of an abrupt transition from zero to finite evaporation assumed in G07 and JGP09. This is in agreement with results from direct numerical simulations (DNS) discussed in Andrejczuk et al. (2004, 2006) and with simulations using the Explicit Mixing Parcel Model (EMP; e.g., Krueger et al. 1997; Su et al. 1998).

The second issue involves the impact of the subgrid-scale mixing scenario (i.e., homogeneous versus inhomogeneous mixing) on the concentration and size of cloud droplets. The double-moment scheme allows specifying the mixing scenario through the parameter $\alpha$ according to (11) in Morrison and Grabowski (2008); that is,

$$N_i - \Delta N = N_i \left( \frac{q_i - \Delta q^x}{q_c^*} \right)^\alpha,$$

where $q_i$ and $N_i$ are respectively the cloud water mixing ratio and droplet concentration prior to including effects of evaporation due to the subgrid-scale mixing. These values include effects of all other processes, such as the resolved (advective) and parameterized (subgrid scale) transport and the evaporation due to the resolved changes of thermodynamic properties—vertical motion in particular. The term $\Delta q_i$ is the cloud water that needs to evaporate as a result of the subgrid-scale mixing, and $\Delta N$ is the corresponding change of the droplet concentration that depends on the value of $\alpha$. Possible values of $\alpha$ are between 0 (homogeneous mixing; $\Delta N = 0$) and 1 (extremely inhomogeneous mixing; $\Delta N = N_i/\Delta q_i^x$). Note that $\Delta q_i^x$ and $\alpha$ in (1) still need to be specified.

The above two issues are related because if cloud water evaporation is delayed entirely until $\lambda = \lambda_0$, then the mixing should only be homogeneous because all droplets are then exposed to the same conditions. In other words, the issue of the homogeneous versus inhomogeneous mixing exists only if some of the cloud water is allowed to evaporate before $\lambda$ reaches the homogenization-scale $\lambda_0$. The next section explains how these two issues are systematically considered in order to develop a consistent framework to represent microphysical transformations due to turbulent mixing in the double-moment warm-rain microphysics scheme.

a. Evaporation of cloud water during turbulent stirring

At each model time step and for a grid box with $\lambda_0 < \lambda < \Lambda$, the amount of the cloud water that has to evaporate because of subgrid-scale mixing over a time step can be estimated in the following way. As in G07 and JGP09, $\Lambda$ is the spatial scale of the initial engulfment of entrained air that undergoes subgrid-scale turbulent mixing, assumed to be equal to the model horizontal grid length. On the cloud microscale, the evaporation of cloud water during the stirring phase occurs at the interface
separating cloudy and cloud-free air [see discussions in Grabowski (1993) and Andrejczuk et al. (2004, 2006)]. The overall strategy is to estimate the area of this interface during turbulent stirring, and to consider processes occurring near the interface. We follow the ideas developed in Sreenivasan et al. (1989) for the general case of mixing in turbulent flows, and subsequently adapted to the case of entrainment and mixing in shallow convective clouds by Malinowski and Zawadzki (1993).

The area of the interface \( S \) corresponding to \( \lambda \) can be estimated in the following way. Assuming that the volume of the cloudy air is \( V_\lambda = \lambda S_\lambda \) and noting that the bulk model predicts \( V_\lambda = \beta \lambda^3 \) leads to

\[
S_\lambda = \frac{\beta \lambda^3}{\lambda}.
\]

(2)

It follows that the surface area separating the cloudy and cloud-free air increases as \( 1/\lambda \) when \( \lambda \) decreases during the stirring phase of the turbulent mixing.

Another way of estimating \( S_\lambda \) is based on the discussion in Sreenivasan et al. (1989) and Malinowski and Zawadzki (1993). The interface is assumed to have fractal properties with the fractal dimension \( D \) (\( 3 > D > 2 \)), and its area \( S_\lambda \) is given by

\[
S_\lambda = S_\lambda \left( \frac{\lambda}{\lambda_0} \right)^{D-2} = a \lambda^D \lambda^{2-D},
\]

(3)

where \( a \lambda = a \lambda^2 \) is the surface of the initial engulfment. Combining (2) and (3) and rearranging terms gives

\[
a = \beta (1/\lambda)^{D-3}.
\]

Note that (3) gives physically consistent expressions for \( S_\lambda \) during the initial engulfment (i.e., \( S_\lambda = S_\lambda = \beta \lambda^2 \) for \( \lambda = \lambda_0 \)), as well as just before microscale homogenization [i.e., for \( \lambda = \lambda_0 \) cf. (2.2) in Sreenivasan et al. (1989) and (1) in Malinowski and Zawadzki (1993)].

Having estimated the interface surface area, we are now ready to estimate the microscale transport across the interface that determines the amount of cloud water that evaporates at the cloud microscale during the stirring phase. For the case of turbulent mixing involving molecular diffusion only, Sreenivasan et al. (1989) first provide an estimate of the depth of the interface across which the molecular diffusion takes place (equal to the Kolmogorov microscale; see p. 86 therein) and then estimate the diffusional transport across this interface [see (2.6) therein]. However, evaporation of cloud droplets near the cloud–clear-air interface is a more complicated problem involving the diffusion of water vapor and temperature across the interface as well as sedimentation of cloud droplets from cloudy into cloud-free air [see discussions in Grabowski (1993), Fig. 3 in section 3 in particular, and Andrejczuk et al. (2004, 2006)]. These processes depend on thermodynamic properties of the cloudy and clear air (e.g., temperature and moisture on both sides of the interface, concentration and sizes of cloud droplets, etc.) and only some of these are predicted by the model. It follows that designing a robust approach that takes all these processes into account is difficult.

Instead, we propose a simpler approach based on the following discussion. First, we assume that, during the model time step, the cloud water \( \Delta q_e^* (>0) \) that evaporates near the interface is a fraction of the cloud water \( \Delta q_e \) that would evaporate during the model time step in a traditional model—that is, when the microphysical adjustment is applied without any delay due to subgrid-scale considerations. Note that \( \Delta q_e \) includes only evaporation associated with parameterized subgrid-scale transport and numerical diffusion. Thus, we postulate that \( \Delta q_e^* = K \Delta q_e \), where the coefficient \( K \) should depend on \( \lambda \), reflecting the increase of \( S_\lambda \) when \( \lambda \) decreases. The main advantage of such a heuristic assumption is that \( \Delta q_e^* \) is tied to the mean thermodynamic properties of the model grid box without considering details of the distribution of these variables inside cloudy and clear-air fractions of the grid box.

A specific expression for \( K \) can be proposed based on the following discussion. Since the evaporation \( \Delta q_e^* \) takes place along the interface separating the cloudy and clear air, the volume affected by the evaporation is approximately \( S_\lambda d \), where \( d \) is the depth of a layer near the interface affected by the evaporation. Arguably, \( K \) should be approximately equal to the ratio of the volume \( S_\lambda d \) to the volume occupied by the cloudy air \( S_\lambda \lambda \) in the ratio is equal to \( d/\lambda \), which implies \( K \approx d/\lambda \). However, when microscale homogenization is already achieved (i.e., \( \lambda = \lambda_0 \)), then \( \Delta q_e^* = \Delta q_e \). It follows that \( K \rightarrow 1 \) when \( \lambda \rightarrow \lambda_0 \), so \( d \) should be taken as \( \lambda_0 \), which gives

\[
\Delta q_e^* = \frac{\lambda_0}{\lambda} \Delta q_e.
\]

(4)

Once \( \Delta q_e^* \) is known, then it can be used to calculate the change of the droplet concentration due to evaporation according to (1). Note that in SGPM12, \( \Delta q_e \) was calculated by explicitly considering subgrid-scale transport terms for the temperature and moisture. A different approach is used here. The total evaporation of cloud water is first partitioned between the adiabatic part (approximated by \( \beta C_{ad} \Delta t \), where \( C_{ad} \) is the adiabatic condensation rate and \( \Delta t \) is the model time step) and the remainder, with the latter assumed to represent \( \Delta q_e \). Such an approach includes into \( \Delta q \) not only explicit subgrid-scale transports but also numerical diffusion.
Finally, $\Delta q^b_\beta$ is associated with the reduction of the original $\beta$ into $\beta'$:

$$\beta' = \frac{q_c - \Delta q^b_\beta}{q_c} \beta,$$  \hspace{1cm} (5)

where $q_c$ is the cloud water mixing ratio in the grid box before the evaporation. Corresponding reduction of the filament scale from $\lambda$ to $\lambda'$ involves $D$ because $\beta/\beta' = (\lambda/\lambda')^{3-D}$. This is derived by combining (2) and (3) and solving for $\beta$. It follows that

$$\lambda' = \lambda \left( \frac{\beta'}{\beta} \right)^{1/(3-D)} \approx \lambda \left( \frac{\beta'}{\beta} \right)^{2.2},$$  \hspace{1cm} (6)

since, according to Malinowski and Zawadzki (1993), $D \approx 2.55$. Thus, (5) and (6) define additional sinks of $\lambda$ and $\beta$ in the $\lambda - \beta$ scheme.

b. Local prediction of the homogeneity of mixing

The homogeneity of mixing (i.e., the value of $\alpha$) depends on relative magnitudes of the local time scales for droplet evaporation and turbulent homogenization. We take advantage of an analysis of a large set of DNS reported in Andrejczuk et al. (2009). Andrejczuk et al. (2009) performed 72 simulations of decaying moist turbulence mimicking turbulent mixing and microscale homogenization of cloudy and clear air using detailed (bin) microphysics. The results were analyzed in terms of the instantaneous change of microphysical characteristics versus the ratio between the turbulent mixing and droplet evaporation time scales. The two scales were derived using parameters describing the progress of the turbulent stirring, such as the spatial scale of cloudy filaments and the turbulent kinetic energy (TKE), as well as the mean size of cloud droplets and the mean relative humidity of cloud-free air within the DNS domain. These parameters can be derived from variables predicted by the LES model by applying the $\lambda - \beta$ scheme as explained below.

The turbulent homogenization time scale, following Andrejczuk et al. (2009), is approximated by the eddy turnover time (e.g., Jensen and Baker 1989):

$$\tau_{\text{mix}} = \lambda/u(\lambda),$$  \hspace{1cm} (7)

where $u(\lambda)$ is the characteristic velocity at $\lambda$. It can be related to the model-predicted subgrid-scale TKE ($E$) as $u(\lambda) = E^{1/2}(\lambda/\lambda)^{1/3}$. This relationship assumes the inertial range scaling for subgrid-scale turbulence and considers subgrid-scale TKE to be dominated by eddies of scale $\Lambda$ [i.e., $u(\Lambda) \approx E^{1/2}$].

The droplet evaporation time scale is estimated as

$$\tau_{\text{evap}} = \frac{r^2}{A(1 - RH_d)},$$  \hspace{1cm} (8)

where $r$ is the mean volume radius of the cloud droplets, $RH_d$ is the relative humidity of the cloud-free portion of the grid box, and $A \approx 10^{-10} m^2 s^{-1}$ is the constant in the droplet diffusional growth equation (i.e., $dr/dt = AS/r$, where $S = RH - 1$ is the supersaturation). $RH_d$ can be estimated using the mean (model predicted) relative humidity of a gridbox RH assuming that the cloudy part of the grid box is saturated and has the same temperature as the cloud-free part. These assumptions lead to

$$RH_d = \frac{RH - \beta}{1 - \beta}.$$  \hspace{1cm} (9)

The change of the microphysical characteristics in Andrejczuk et al. (2009) was measured by the slope $\delta$ of the line depicting evolution of the total number of droplets plotted against the mean volume radius cubed, both normalized by the initial values, applied in Andrejczuk et al. (2004, 2006) and referred to here as the $r^3 - N$ diagram.\footnote{The $r^3 - N$ diagram is similar to the diagram used in Burnet and Brenguier (2007), but it applies the number of droplets involved in DNS of the turbulent mixing rather than the droplet concentration derived from aircraft observations used in Burnet and Brenguier (2007). The main difference is a simpler representation of the homogeneous mixing on the $r^3 - N$ diagram.} In the $r^3 - N$ diagram, homogeneous mixing corresponds to a horizontal line (i.e., changing droplet size without changing the number of droplets; $\delta = 0$), whereas a vertical line (reduction of the number of droplets without changing the size; $\delta \rightarrow \infty$) implies extremely inhomogeneous mixing [see examples in Fig. 1 in Andrejczuk et al. (2009)]. Based on these simulations, Andrejczuk et al. (2009) proposed a simple relationship between the ratio of the two time scales and the slope of the mixing line of the $r^3 - N$ diagram [see Fig. 2 in Andrejczuk et al. (2009)]. Because of a significant scatter among DNS results and limitations of Andrejczuk et al. (2009) DNS model (e.g., a relatively narrow range of spatial scales and the domain size much smaller than the LES grid box), we simplify the relationship suggested in Andrejczuk et al. (2009) and assume that $\delta$ is equal to the ratio between time scales of turbulent homogenization and of droplet evaporation; that is, $\delta = \tau_{\text{mix}}/\tau_{\text{evap}}$.

The slope is related to the parameter $\alpha$ in (1) through the following argument. Because $q_c \sim N \rho^3$, (1) implies that $N \sim (r^3 \rho^3)^{(1-\alpha)/\alpha}$. Linearization of this relationship gives the slope $\delta = dN/d(r^3)$ of $\alpha/(1 - \alpha)$, which leads to
\[
\alpha = \frac{\delta}{1 + \delta}.
\] (10)

Once the values of the two time scales are derived using (7) and (8), their ratio provides a prediction of \(\delta\), and the homogeneity of \(\alpha\) can be calculated from (10) and applied in (1).

The entire algorithm that merges the \(\lambda - \beta\) model with the double-moment warm-rain microphysics can be summarized as follows. For a grid box with either \(\lambda = \Lambda\) or \(\lambda = 0\)—that is, either homogeneous cloudy or cloud free, respectively—evaporation and condensation are calculated as in the traditional double-moment scheme. For a grid box with \(\lambda_0 < \lambda < \Lambda\), the expected evaporation or condensation of cloud water \(\delta q_c\) is calculated first using the grid-averaged fields. If condensation is predicted to occur, then as in G07 the grid is assumed homogeneous, and \(\delta q_c\) is applied in the microphysics scheme, \(\lambda\) is reset to \(\Lambda\), and \(\beta\) is reset to 1. For the evaporation, \(\delta q_c\) is first partitioned into the adiabatic part \(\beta C_{\text{ad}} \Delta t\) and the \(\Delta q_t\) part (assuming \(\delta q_c = \beta C_{\text{ad}} \Delta t - \Delta q_t\), since \(\Delta q_t\) is assumed positive). The latter combines explicit (resulting from calculated subgrid-scale turbulent mixing terms) and implicit (numerical) diffusion. Subsequently, only a fraction of \(\Delta q_t\), \(\Delta q_t^* = \lambda_0 \Delta q_t / \lambda\), is allowed to evaporate as given by (4), with the evaporation affecting droplet concentration as implied by (1) and the parameter \(\alpha\) calculated as described above. In addition, \(C_{\text{ad}}\) is applied to the \(\beta\) fraction of the grid box assuming no change in droplet concentration. When microscale homogenization is reached (i.e., \(\lambda = \lambda_0\)), \(\lambda\) is reset to \(\Lambda\) and \(\beta\) is reset to 1.

3. Model setup and model simulations

Developments presented in the previous section were added to the numerical model used in SGPM12. The model is based on the 3D anelastic semi-Lagrangian–Eulerian model (EULAG) documented in Smolarkiewicz and Margolin (1997, model dynamics), Grabowski and Smolarkiewicz (1996, model thermodynamics), and Margolin et al. (1999, subgrid-scale turbulent mixing). Prusa et al. (2008) provide a recent review with comprehensive list of references. EULAG is set up as an LES model to simulate steady-state trade wind shallow convection observed during BOMEX (Holland and Rasmusson 1973) and used in the model intercomparison study described in Siebesma et al. (2003). In the BOMEX case, the 1.5-km-deep trade wind convection layer overlays a 0.5-km-deep mixed layer near the ocean surface and is capped by a 0.5-km-deep trade wind inversion layer. The cloud cover is about 10% and quasi-steady conditions are maintained by the prescribed large-scale subsidence, large-scale moisture advection, surface heat fluxes, and radiative cooling. As in Siebesma et al. (2003), the model is run for 6 h, and results from the last 3 h are used in the analysis. Although the design of the BOMEX case targets nonprecipitating trade wind shallow convection, we keep the warm-rain parameterization active. This leads to a small autoconversion of the cloud water into rain, with trace (small) rainwater mixing ratios near the tops of the tallest clouds in polluted (pristine) simulations.

The only difference between the model setup proposed in Siebesma et al. (2003) and used here is a reduction of the horizontal (vertical) grid length from 100 (40) to 50 (20) m, keeping the same number of grid points in horizontal directions. Such a change is similar to that used in JGP09 and SGPM12 and leads to a smaller computational domain compared to Siebesma et al. (2003). This is dictated by the need to appropriately represent cloud-base activation, although the 20-m vertical grid length is still fairly coarse [see discussion in section 4 in Morrison and Grabowski (2008)]. As in Morrison and Grabowski (2007, 2008) and SGPM12, we contrast results obtained assuming either the maritime aerosol characteristics with the total CCN concentration of 100 mg^{-1} (referred to as pristine) or the continental aerosol characteristics with CCN concentration of 1000 mg^{-1} (the polluted case). These values are used in the CCN activation scheme as described in section 2a of Morrison and Grabowski (2007) with all other parameters characterizing the aerosol exactly as described there.

Five simulations are performed for each of the two aerosol conditions—that is, 10 simulations altogether. The first set of two simulations (i.e., for pristine and polluted aerosol) includes all developments discussed in section 2; that is, it includes the delay of cloud water evaporation resulting from the subgrid-scale mixing and the local prediction of \(\alpha\) that characterizes homogeneity of the mixing. Most of the results presented in the paper come from these two simulations. We also include two sets of sensitivity simulations, each consisting of four simulations. The first set includes simulations for polluted and pristine aerosol where the homogeneity of mixing is prescribed as in SGPM12—that is, with either \(\alpha = 0\) or \(\alpha = 1\). An important difference from SGPM12 simulations is that prescribed-\(\alpha\) simulations in this set include the delay of cloud water evaporation due to mixing. In other words, these simulations include all developments presented in this paper, except that the fixed \(\alpha\) is used instead of the locally predicted value. The second set of four sensitivity simulations also applies either \(\alpha = 0\) or \(\alpha = 1\) for polluted and pristine aerosol, but the delay of cloud water evaporation due to mixing is suppressed; that is, the locally predicted \(\lambda\) is replaced by \(\lambda_0\) in (4). The prescribed-\(\alpha\) simulations from this set are...
as in SGPM12, except that the subgrid-scale transport contribution to the cloud water evaporation is calculated differently as explained above.

Snapshots of model fields saved every 3 min are used in the analysis of model results. Statistics of conditionally sampled snapshots averaged in time for the last 3 h of the simulation will mostly be used.

4. Results

a. Macroscopic cloud-field characteristics

As far as macroscopic cloud-field characteristics are concerned, results from simulations reported in this paper are in agreement with those presented in SGPM12. For instance, the cloud fraction profiles feature a maximum of about 8% near the cloud base at around 0.5 km, a rapid decrease to about 3% at 1.0 km, then a more gradual decrease to about 2% at 1.5 km, and finally reach 0% at around 2 km. The profiles are also similar to those presented in Fig. 6 of Siebesma et al. (2003), but with 1%–2% higher values between the cloud base and the height of 1.5 km. The difference profiles between various simulations herein are also similar to those shown in SGPM12 (cf. Fig. 1 therein), with typical difference values smaller than 0.5%. Larger differences, reaching about 1% at around 0.7 km, are for simulations without the delay of cloud water evaporation. These are consistent with the differences between simulations with and without the delay reported in G07. However, cloud-field depth is the same in simulations with and without the delay of cloud water evaporation associated with subgrid-scale mixing, which is in contrast to results presented in G07 and JGP09. The latter difference might be due to the intrinsic contrast between the saturation-adjustment bulk thermodynamic scheme applied in G07 and JGP09 and the scheme that predicts in-cloud super-saturation and features a finite-droplet-evaporation time scale used here.

Numerical simulations of Xue and Feingold (2006) suggest that the difference of the mean cloud droplet radius within shallow convective clouds developing in pristine and polluted environments affects the rate of entrainment-related evaporation of cloud droplets and subsequently such macroscopic cloud-field characteristics as the cloud fraction and the domain-averaged cloud water and vertical velocity variance (see Figs. 2, 4, 6, and 7 therein). This conjecture is also supported by aircraft observations reported in Small et al. (2009). Analysis of current simulations provides inconclusive results. The cloud-fraction profiles differ little as mentioned above, but indeed smaller cloud fractions are predicted for the polluted conditions in the upper half of the cloud-field depth. The domain-averaged cloud water for the polluted conditions is smaller compared to the pristine case, but significantly less so than in Fig. 6 of Xue and Feingold (2006). The variance profiles differ little as well, which is in contrast to the results shown in Fig. 7 of Xue and Feingold (2006). It is unclear if the overall discrepancy comes from a significantly smaller contrast between pristine and polluted conditions considered here and in Xue and Feingold (2006) (CCN concentrations of 100 versus 1000 mg$^{-1}$ herein and 25 versus 2000 mg$^{-1}$ therein) or from the delay of the entrainment-related evaporation included in the model used in the current study.

b. Mixing characteristics

Figure 1 shows the contoured frequency by altitude diagrams (CFADs) of $\alpha$ from pristine and polluted simulations. Only points with cloud water mixing ratio larger than 0.01 g kg$^{-1}$ are taken into account, and levels where the number of data points is smaller than 0.2% of the total number of data points at the level are excluded. The latter is to avoid levels with a small number of data points that make the frequency plots noisy (this typically happens near the top of the cloud field where clouds are able to penetrate only very infrequently). CFADs document in a comprehensive way statistical distributions of quantities simulated by the model at a given height. The panels also show profiles of the mean values as solid lines; the dashed line shows the mean from the neighboring panel to highlight the difference between pristine and polluted cases.

Figure 1 shows that the range of simulated mixing scenarios at a given height within the field of shallow cumuli is wide, from close to homogeneous ($\alpha = 0$) to near extremely inhomogeneous ($\alpha = 1$). The mean characteristics shift toward homogeneous mixing with height. At any given height, the mean mixing scenario is shifted toward homogeneous mixing in the pristine case when compared to the polluted.

The homogeneity of the subgrid-scale mixing depends on the mixing and evaporation time scales $\tau_{\text{mix}}$ and $\tau_{\text{evap}}$. CFADs of the two time scales are shown in Figs. 2 and 3 in the same format as Fig. 1. Only cloudy points where subgrid-scale mixing takes place are included in the analysis. The distributions of the mixing time scale (Fig. 2) are relatively wide, from 1 s or less to 100–200 s, with the mean and the width decreasing with height. The differences between pristine and polluted conditions are relatively small. The top of the cloud-field features strongly skewed distributions, with most of the points having relatively small values. The evaporation time scale (Fig. 3) shows similar features (wide distributions, highly skewed near the cloud-field top), with the mean
values approximately constant with height—around 70 and 30 s for the pristine and polluted cases, respectively. This difference between cases leads to more homogeneous mixing in the pristine case as shown in Fig. 1. The figures explain the height dependence of the mean mixing characteristics (i.e., the mean $\alpha$) documented in Fig. 1 because the mean value of $\tau_{\text{evap}}$ changes with height insignificantly, and the mean value of $\tau_{\text{mix}}$ decreases with height, thus favoring more homogeneous mixing aloft. The significant spread of the time-scale distributions leads to a large variability of the local mixing characteristics evident in Fig. 1.

The turbulent mixing time scale is a function of subgrid-scale turbulent kinetic energy and the scale of cloudy filaments: $\tau_{\text{mix}} \sim \lambda^{2/3}E^{-1/2}$ [see (7)]. CFADs of these variables are shown in Figs. 4 and 5. CFADs of $E$ are highly skewed, with the majority of points having values around a few hundredths of $1 \text{ m}^2 \text{s}^{-2}$ and a mean around $0.1 \text{ m}^2 \text{s}^{-2}$. The width of the distribution increases with height, and so does the mean value, especially above 1.5 km. Because the TKE formulation in the model does not explicitly consider microphysical effects on the $E$ production (Margolin et al. 1999), profiles of $E$ in pristine and polluted cases are virtually the same.

Figure 5 presents CFADs of $\lambda$ as predicted by the model in pristine and polluted simulations. The distributions are relatively wide and highly skewed, especially in the upper parts of the cloud field. Mean $\lambda$ weakly

FIG. 1. CFADs of $\alpha$ for simulations of (a) pristine and (b) polluted cases. Solid lines show the average vertical profiles; analogical profiles from the other panel are shown using a dashed line. Only cloudy points where subgrid-scale mixing takes place are included.

FIG. 2. CFADs of $\tau_{\text{mix}}$ for simulations of (a) pristine and (b) polluted cases. Solid lines show the average vertical profiles; analogical profiles from the other panel are shown using a dashed line. Only cloudy points where subgrid-scale mixing takes place are included.
decreases with height. The differences between polluted and pristine clouds are relatively small. Overall, Figs. 4 and 5 show that the decrease of the mean value of $\tau_{\text{mix}}$ with height (Fig. 2) comes from the combination of the increase of the mean TKE and the decrease of the mean $\lambda$.

The evaporation time scale depends on the size of cloud droplets and the relative humidity of the cloud-free portion of the gridbox: $\tau_{\text{evap}} \sim r^2 (1 - RH_d)^{-1}$ [see (8)]. In contrast to $E$ and $\lambda$, CFADs of the mean volume radius (Fig. 6) differ significantly between pristine and polluted cases. This is especially true for the mean radius, which increases with height in both cases and is centered at values around 10 $\mu$m for the pristine case and around 6 $\mu$m for the polluted case. Note that there is a wide range of droplet radii near the cloud base; then the distribution narrows significantly (with the minimum around 0.7 km), only to increase in width higher up. This peculiar feature near the cloud base most likely comes from the presence of very shallow weak-updraft clouds that do not reach the level of free convection and only mark the uppermost edges of boundary layer eddies. Arguably, activation of CCN in those clouds is poorly resolved with the 20-m vertical grid length and this leads to very low droplet concentrations and unrealistically large sizes.

Figure 7 shows CFADs of relative humidity $RH_d$ in the cloud-free fractions of grid boxes undergoing
turbulent mixing that affects $\tau_{\text{evap}}$. The figure shows that RH$_d$ is high, typically above 95%, and often 99%. As one might expect, the pristine case has slightly lower RH$_d$, arguably because of larger cloud droplets and their slower evaporation. The decrease of the mean RH$_d$ with height counteracts the increase of the mean droplet radius (see Fig. 6) and results in approximately constant mean $\tau_{\text{evap}}$ with height (Fig. 3).

c. Results from sensitivity simulations

Sensitivity simulations of polluted and pristine conditions show results in general agreement with the above discussion. When the delay of cloud water evaporation is allowed as in the main pair of simulations discussed above, the differences between prescribed-$\alpha$ simulations and simulations discussed in the previous section are small—even smaller than in SGPM12. The lack of the impact of the mixing scenario can be understood by considering factors affecting subgrid-scale mixing characteristics—RH$_d$ in particular. As Fig. 7 shows, RH$_d$ is typically high—above 95%—and the same is true for sensitivity simulations (not shown). SGPM12 argued (based on a simple model of bulk entrainment) that the air entrained into a cloud and involved in the small-scale mixing is indeed quite humid and thus little
evaporation of cloud droplets is needed. Current results provide strong support for this conjecture. The relative humidity of the cloud layer unperturbed environment is relatively high in the BOMEX case—above 90% at the cloud base and decreasing to 75% at 1.5 km. The air entrained into a cloud is even more humid because it comes from a cloud halo (e.g., Perry and Hobbs 1996; Lu et al. 2002), as more recently documented in numerical simulations and aircraft observations discussed in Jonker et al. (2008), Heus et al. (2009), and JGP09 (see Fig. 4 therein).

As explained in the description of the scheme, the current approach applies a different method to derive the mixing-related cloud water evaporation than was used in SGPM12. The mixing-related evaporation rate combines the parameterized transports with the transport (and evaporation) due to numerical diffusion. SGPM12 suggested that the small difference between simulations assuming either the homogeneous mixing or the extremely inhomogeneous mixing (i.e., either \( \alpha = 0 \) or \( \alpha = 1 \), respectively, uniformly in space and time) was because the subgrid-scale turbulent mixing contributed little to the mixing between a cloud and its environment when compared to the implicit numerical diffusion (see a computational example and accompanying discussion in the appendix of SGPM12). To support such a conjecture, we performed a set of simulations in which evaporation of cloud water was allowed to proceed as in a traditional model (i.e., the delay of evaporation was excluded by assuming \( \Delta q_{c} = 0 \)).

Prescribed mixing scenarios with \( \alpha = 0 \) and \( \alpha = 1 \) were used as in SGPM12 in the mixing-related part of the total cloud evaporation. Hence, the only difference between these sensitivity simulations and simulations in SGPM12 is the partitioning of the total evaporation rate into the adiabatic part (i.e., the one unaffected by the mixing characteristics) and the one due to subgrid-scale mixing. Sensitivity simulations indeed show that the differences between prescribed-\( \alpha \) simulations without the delay of evaporation are significantly larger. For instance, the mean droplet concentration differs on average 10%–20% across the entire depth of the cloud field in pristine and polluted simulations (not shown). Significant differences between sensitivity simulations with and without the delay of the cloud water evaporation imply that delaying droplet evaporation in the current approach leads to an even smaller impact of the mixing homogeneity than in SGPM12.

5. Analysis of model results in the context of aircraft observations

Prediction of the local subgrid-scale mixing characteristics allows analysis of the relationship between macro- and microphysical features of simulated small cumulus clouds and comparison with field observations. This section discusses results of such an analysis and focuses on selected heights in contrast to the height-dependent statistics presented previously.

Figure 8 presents a scatter diagram of \( \alpha \) versus the adiabatic fraction (AF) (i.e., the ratio between the local LWC and its adiabatic value) at a height of 1.0 km—that is, about 450 m above the cloud base—for the pristine case. The adiabatic fraction considers the fraction of gridbox volume occupied by the cloudy air; that is, the local LWC is defined as the model-predicted LWC
divided by $\beta$. For clarity, only every tenth data point from all clouds and for snapshots from the last 3 h of the simulation is plotted. Plots of the polluted case and for other heights are similar, except for a shift toward more inhomogeneous mixing for the polluted case and a slight shift toward more homogeneous mixing with increasing height, which is in agreement with the data presented in Fig. 1. The figure shows that the range of mixing scenarios narrows as AF increases: it features almost the entire range of $\alpha$ for low AF and approaches $\alpha \sim 0.3$ for the largest AF encountered at this height. The mean mixing scenario shifts toward extremely inhomogeneous mixing with AF approaching small values, which is a trend suggested by cloud observations discussed in Burnet and Brenguier (2007) and Lehmann et al. (2009). The decrease in the number of points with increasing AF is consistent with the fact that shallow cumuli are strongly diluted and it is difficult to find high values of AF as one moves upward in the cloud field.

Figure 8 only includes cloudy points where $\alpha$ is calculated—that is, points undergoing cloud–environment mixing. In contrast, Fig. 9 includes all cloudy points for the pristine simulation at the same level. The figure shows a scatter diagram of the model-predicted droplet concentration $N$ versus the local concentration in the cloudy part of the grid box $\frac{N}{\beta}$. As in Fig. 8, only every tenth data point is included in the plot. The left (right) panel applies a color scale to indicate AF (vertical velocity $w$) within the grid box. The figure shows that grid boxes are typically uniform (i.e., $\beta = 1$) for droplet concentrations larger than about $40 \text{ mg}^{-1}$—that is, about the half of the maximum adiabatic droplet concentration (which is close to $90 \text{ mg}^{-1}$ for the pristine case). The highest droplet concentrations are observed in cloudy parcels with the highest AF and highest $w$ at this level. Grid boxes with lower droplet concentrations and lower AF but with $\beta = 1$ represent cloudy volumes that were previously diluted by entrainment but that have since become uniform (i.e., fully cloudy). Such cloudy volumes may experience enhanced growth of cloud droplets (i.e., the mean radius may increase faster with height when compared to a parcel with higher droplet concentration) if they move upward. However, the right panel shows that this is unlikely as such diluted and uniform volumes are typically in regions of reduced vertical velocity, most likely near cloud edges. Grid boxes with mean droplet concentrations smaller than about $40 \text{ mg}^{-1}$ are typically significantly diluted and nonuniform, and the differences between the mean and local concentrations are large. Local droplet concentration

![Figure 8](image-url)

**Fig. 8.** Scatter diagram of $\alpha$ vs AF at the height of 1.0 km for the pristine case. The local LWC is defined as the model-predicted LWC divided by $\beta$. Solid line marks average $\alpha$.

![Figure 9](image-url)

**Fig. 9.** Scatter diagram of $N$ vs $\frac{N}{\beta}$ at the height of 1.0 km for the pristine case. Color scale is applied to indicate (left) AF and (right) $w$ within the grid box.
in such volumes may be unresolved by aircraft observations [see Paluch and Knight (1984); section 3.3 in Lu et al. (2011) and references therein]. Positive correlation between the droplet concentration and adiabatic fraction evident in the left panel is consistent with aircraft observations (e.g., Austin et al. 1985).

Figure 10 shows the diagram introduced in Burnet and Brenguier (2007) and subsequently used in observational cloud studies focusing on the microphysical structures of clouds (e.g., Lehmann et al. 2009). The figure shows a scatter diagram of the mean volume radius of cloud droplets cubed \( r_\nu^3 \) versus the mean local droplet concentration at the same height as Figs. 8 and 9. The left (right) panel uses color to depict the local updraft velocity (local value of \( \alpha \)); only every third data point is included in the plot. The right panel includes only points where \( \alpha \) is calculated—that is, a subset of cloudy points shown in the left panel. Black lines show isolines of LWC and the dashed line represents adiabatic LWC at this height. Red lines represent extremely inhomogeneous mixing. Blue lines represent homogeneous mixing with the air of the same temperature and relative humidity of 98%. Two starting points were selected for the red and blue mixing lines.

Overall, the data points included in Fig. 10 form a pattern resembling that from aircraft observations of shallow convective clouds discussed in Burnet and Brenguier (2007, Figs. 8b,c therein) and Lehmann et al. (2009, Figs. 5a,b therein). In addition, the figure shows that LWC close to adiabatic is associated with the largest vertical velocities (red colors in the left panel), as one might anticipate. Colors representing significant updrafts in the left panel seem to be aligned in vertical belts; that is, they represent similar droplet concentrations across a range of LWC. For instance, the red color corresponds to the volumes with the droplet concentrations of about 80 mg \( \cdot \) m\(^{-3}\) and a range of LWC between 0.7 and 1.0 g kg\(^{-1}\). Concentrations associated with these belts increase with the increasing vertical velocity, as one might expect from the dependence of droplet activation on the vertical velocity (at the cloud base as well as aloft because of in-cloud activation). Note that these belts are absent in the right panel, which implies that they are uniform (\( \beta = 1 \)) despite being diluted by entrainment. The close-to-vertical alignment of these belts can be interpreted as resulting from previous close-to-homogeneous mixing (i.e., significant reduction of LWC accompanied by a small decrease of the concentration). Another interpretation might be that these points represent volumes in which extremely inhomogeneous

\[ \frac{r_\nu^3}{N/\nu} \text{ at height of 1.0 km for the pristine case. Color is applied to depict (left) local updraft velocity and (right) local value of \( \alpha \). The right panel includes only points where \( \alpha \) is calculated—that is, a subset of cloudy points shown in the left panel. Black lines show isolines of LWC and the dashed line represents adiabatic LWC at this height. Red lines represent extremely inhomogeneous mixing. Blue lines represent homogeneous mixing with the air of the same temperature and relative humidity of 98%. Two starting points were selected for the red and blue mixing lines.} \]
mixing is followed by significant in-cloud activation. Such a chain of events also results in the reduction of LWC and high droplet concentration. The significance of in-cloud activation is strongly supported by the sheer number of data points to the right of the homogeneous mixing line. In fact, one can argue that it is difficult to distinguish earlier episodes of homogeneous mixing from episodes of inhomogeneous mixing followed by in-cloud activation in diagrams like Fig. 10. Krueger (2008) provides in-depth analysis of various cloud processes (entrainment and isobaric mixing, CCN activation, condensational growth, etc.) are mirrored on diagrams like the one shown in Fig. 10.

Data points in the right panel (i.e., those undergoing turbulent stirring) typically correspond to vertical velocities close to zero or negative, with the strongest downdrafts corresponding to the most diluted volumes. The local mixing scenario seems to change from more homogeneous at higher LWC (blue colors) toward more inhomogeneous at lower LWC (red colors), which is in agreement with data shown in Fig. 8 and observations reported in Lehmann et al. (2009). Based on previous studies (Burnet and Brenguier 2007; Lehmann et al. 2009), one might suggest that points undergoing turbulent stirring represent effects of the homogeneous mixing because they seem to be aligned along the blue lines. However, the figure shows that such an interpretation is generally not correct because a wide range of local mixing scenarios is simulated by the model, as shown by the range of colors in the right panel. One has to keep in mind, however, that the local mixing scenario may not reflect history of past mixing events (i.e., along air trajectories arriving at the level from which data points are taken) that ultimately determine microphysical characteristics of a given cloudy volume (see also Krueger 2008). Similar diagrams for the polluted case and for different heights provide results broadly consistent with the above discussion, except for obvious trends due to differences between pristine and polluted clouds (e.g., smaller droplet sizes in the latter case) and systematic decrease of the mean adiabatic fraction with height.

Overall, Figs. 8–10 provide useful insights into the interaction between macro- and microphysical processes in shallow convective clouds. The analysis complements results of aircraft observations discussed in Burnet and Brenguier (2007) and Lehmann et al. (2009), among others.

6. Discussion and summary

This paper presents an approach that allows local prediction of the homogeneity of subgrid-scale turbulent mixing in large-eddy simulation of warm (i.e., ice-free) clouds. Because warm clouds are close to water saturation, conservation of the total water and moist static energy allows an accurate prediction of the temperature, water vapor, and cloud water mixing ratios of the homogenized mixture. However, predicting the change of the droplet spectrum requires additional constraints because the same amount of cloud water after homogenization can be distributed over droplet spectra that differ significantly (e.g., reduced droplet concentration versus reduced mean size when compared to the undiluted cloudy air). Predicting the change of the droplet size and concentration after homogenization is the essence of the subgrid-scale mixing scenario. Homogeneous mixing involves reduction of the mean droplet size with no change of the number of droplets from evaporation (the dilution due to entrainment leads to some reduction of the droplet concentration). In contrast, extremely inhomogeneous mixing involves reduction of the droplet concentration without any change of the mean droplet size. These two scenarios provide limits of what is expected in natural clouds. Because shallow convective clouds are strongly diluted by entrainment, the mixing scenario could significantly affect microphysical cloud characteristics, such as the mean droplet radius and the mean droplet concentration. These, in turn, affect the ability of clouds to produce precipitation and impact cloud optical properties (e.g., cloud albedo).

The mixing scenario depends on the relative magnitudes of two time scales: the time scale of turbulent homogenization and the time scale of cloud droplet evaporation. Homogeneous mixing is thought to occur when turbulent homogenization is significantly faster than the droplet evaporation; in the opposite limit, extremely inhomogeneous mixing is supposed to take place. To locally predict homogeneity of mixing, the approach to delay cloud water evaporation during turbulent stirring [applied previously in the single-moment bulk microphysics with saturation adjustment (G07; JGP09)] was merged with the double-moment warm-rain microphysics scheme of Morrison and Grabowski (2007, 2008). The delay only applies to the evaporation of cloud water that occurs as a result of turbulent mixing between a cloud and its unsaturated environment. In such a case, initially separate volumes of cloudy and cloud-free environmental air undergo gradual filamentation, with progressively increasing evaporation of cloud water during the approach to microscale homogenization. This process (referred to as turbulent stirring) is represented by including an additional model variable—the spatial scale of the cloudy filaments $\lambda$—whose temporal evolution mimics the transition from coarsely mixed cloud–clear-air volume toward microscale homogenization. The double-moment scheme allows
including the entire range of the subgrid-scale-mixing scenarios through changes of a single parameter $\alpha$ [cf. (11) in Morrison and Grabowski (2008) and (1) herein]. A relatively simple procedure is developed here that allows local prediction of $\alpha$ and thus the homogeneity of the subgrid-scale turbulent mixing. Results from a large set of direct numerical simulations of the interfacial mixing (Andrejczuk et al. 2009) are used to link the ratio of the time scales (of turbulent mixing and of droplet evaporation) with $\alpha$.

The new approach is used in simulations of a shallow convective cloud field applied to the BOMEX setup (Siebesma et al. 2003) and contrasting clouds with pristine and polluted CCN characteristics following SGPM12. Model results show that the mixing scenario varies significantly within the simulated cloud field, from close to homogeneous to not far from extremely inhomogeneous. This is because of spatial and temporal variations of local cloud conditions—the intensity of the subgrid-scale turbulence and the mean cloud droplet radius in particular. Statistics of the former do not change between pristine and polluted clouds because subgrid-scale TKE formulation excludes microphysical effects on the subgrid-scale TKE production. The mean droplet radius, however, is significantly larger for the pristine clouds, as one would expect. As a result, statistics of the turbulent homogenization time scale differ little between pristine and polluted cases, but the droplet evaporation time scale is significantly larger (approximately by a factor of 2) for the pristine case. A combination of the two effects leads to mixing characteristics that are on average shifted toward the homogeneous mixing in the pristine case. Moreover, for both pristine and polluted cases, mixing becomes more homogeneous when one moves toward higher levels within the cloud field. This comes from the increase of the mean TKE intensity and the mean droplet radius with height, both favoring more homogeneous mixing.

The lack of differences in statistics between simulations with predicted homogeneity of the subgrid-scale mixing and simulations with prescribed homogeneity (i.e., $\alpha = 0$ or $\alpha = 1$ uniformly in time and space as in SGPM12) suggests that, on average, the homogeneity has an insignificant impact on the mean cloud-field microphysical characteristics, such as the mean volume radius or the droplet concentration. With the delay of mixing-induced evaporation, differences between $\alpha = 0$ and $\alpha = 1$ simulations are smaller than in SGPM12. This is explained as a consequence of the close-to-saturated cloud-free air involved in the turbulent mixing, which implies insignificant differences between various mixing scenarios. Only when the delay of mixing-induced evaporation was excluded (which is physically unjustifiable but assumed in standard LES models; i.e., in SGPM12) did the difference between simulations with prescribed homogeneous and extremely inhomogeneous mixing become more significant than in SGPM12. This difference can be explained by a more appropriate formulation of the subgrid-scale evaporation that includes both the effects of numerical diffusion and explicit subgrid-scale mixing in the approach developed here.

Overall, simulations seem to reproduce selected microphysical features of shallow convective clouds deduced from observations and previous model simulations. A wide range of possible mixing scenarios is consistent with observations reported in Burnet and Brenguier (2007) and Lehmann et al. (2009) and expectations based on spatial and temporal variability of cloud parameters determining mixing homogeneity. Mixing close to homogeneous takes place in volumes with the highest LWC and strongest updraft at a given height—that is, close to the cloud core. Mixing in more diluted volumes is typically close to extremely inhomogeneous. These again agree with observations reported in Lehmann et al. (2009). Cloud volumes with the highest droplet concentrations are typically already homogenized—that is, with cloud fraction $\beta = 1$—and they show the highest LWC at a given height. Volumes with the lowest LWC, much smaller than the adiabatic, typically feature low droplet concentrations, are often heterogeneous (i.e., $\beta < 1$) and occur in regions of a weak updraft or downdraft. Such volumes are expected to feature small-scale structures unresolved by aircraft observations as speculated by Paluch and Knight (1984).

Simulations presented in this paper call for additional studies using the new methodology. First, as shown in JGP99, $\Lambda - \beta$ model results exhibit significant dependence on the model spatial resolution. Second, higher spatial resolution also leads to a better representation of the entrainment, and it is unclear what effect this may have on the subgrid-scale mixing homogeneity. For example, with the conclusion concerning the high relative humidity of the clear air involved in the entrainment and mixing change with higher resolution? With resolved entraining eddies, one might expect that the air involved in the turbulent mixing may be less humid and lead to a more significant impact of the mixing homogeneity. One may also expect that the effects become more significant for clouds developing in a significantly drier environment—for instance, over land. Another aspect not considered in the current study is the role of small-scale intermittency—that is, the subgrid-scale variability of key turbulence characteristics—the dissipation rate in particular. Again, high-spatial-resolution simulations can shed light on this issue. Moreover, the model presented in this paper can also be used to study microphysical
effects of entrainment and mixing in other ice-free shallow cloud systems (cf. Jarecka et al. 2013). Finally, extension of the methodology presented in this paper to the case of the bin microphysics should be considered. All of these aspects warrant additional studies that we hope to report in subsequent publications.

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