D4.3 New model conception (LES/RANS) on interface/droplets interaction

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1 Introduction

Dynamics and lifetime of clouds is strongly connected to the processes at their interface [21]. Entrainment of dry-air results in the reduction of the specific humidity at the cloud boundaries. This leads to enhanced droplet evaporation and a set of further feedback mechanisms. In particular, the important question is how the entrainment influences the spectra of cloud droplets' radii. The width of the spectra, on the other hand are important in the global balances as it has an impact on radiative properties of stratocumulus and shallow convection clouds [14] and determines the onset of gravitational coalescence in warm clouds [3].

The distribution of droplet sizes depends strongly on whether the droplets are exposed to the homogeneous or variable subsaturation [3], which in turn is connected with the characteristic time and length scales of turbulent eddies disrupting the interface. In the complex physical process of entrainment both, the large and the small scales play an important role. Due to the former the cloud/clear air interface undergoes the so-called ”engulfment” which introduces inhomogeneity in the subsaturation field. On the other hand, the influence of the latter is referred to as the small-scale ”nibbling” which mixes and homogenizes the field. In real clouds the range of active scales is enormous - from large hundred meter structures to small eddies of size of millimeter order. Due to insufficient computational powers, numerical modelling of the full spectrum of eddies is currently out of reach. The common practice is either to reduce the size of the computational domain and study the effects of small scales on particle properties with the use of the Direct Numerical Simulations (DNS) [16] or to resolve the large-scale dynamics on the grid with resolution of order of meters, thus truncating the high-wavenumber part of the turbulence spectrum. The latter approach is referred to as Large Eddy Simulation (LES) and requires proper modelling of the influence of unresolved (subgrid) scales.

As classified by [19], there are two essentially different types of closures to account for the effect of turbulence eddies on droplets' dispersion: stochastic and structural. Stochastic models are based on the solutions of the Langevin equations [7, 25] supplemented with a stochastic Wiener process term. Structural sub-grid models aim at reconstructing, in an approximate sense, some of the subgrid turbulent eddies [22]. This allows for tracking the particles (droplets) in the reconstructed fine-grained velocity field. Examples of structural models are the fractal interpolation [28, 18], approximate deconvolution (ADM) [12, 31], spectrally optimized interpolation [13] and the kinematic simulations based on Fourier modes [10, 26]. The present model conception is related to the fractal interpolation technique (FIT). The underlying assumption of the FIT is the existence of fractal-scale similarity of velocity fields. The same scale-similarity has been observed in the structure of cloud/clear-air interfaces [17]. For this reason FIT seems most promising for the modelling of subgrid-scale processes at cloud boundaries. An attribute of the constructed sub-grid velocity depends on the stretching parameter d, which is related to the fractal dimension of the signal. In Scotti and Meneveau [28], it was assumed that d is constant in space and time for homogeneous and isotropic turbulence. Basu et al. [6] extended this work by proposing a bi-valued stretching parameter and showed that it improves resulting statistics. To introduce the new proposal we first argue, based on *a priori* analyses of DNS, LES and experimental data, that the values of the stretching parameter are not constant, but in fact vary significantly in space and time [1]. However, we show that in the inertial range probability density functions (PDFs) of d follow the same, universal profile. For this reason we propose to account for the variability of the stretching parameter, treating d at a given point and time, as a random number with a prescribed, previously determined PDF. We have shown that the approach with random d is the most favourable in terms of the investigated statistics [2]. It reproduces the Kolmogorov's $-5/3$ scaling of turbulent kinetic energy spectra in the inertial range with the smallest error and without spurious modulations. Moreover, PDFs of increments of the reconstructed velocity have non-Gaussian, stretched-exponential tails.

The ultimate goal is to apply the model in the LES of clouds and improve resulting particle statistics at the cloud/clear-air interface. Due to the high computational cost required to simulate clouds dynamics and microphysics, a particle-based model called the super-droplet method was developed by Shima et al [4, 9, 29]. The new sub-grid FIT approach will be used to improve the resolution of the velocity field of the carrier fluid in the coupled Eulerian/Lagrangian model. First simulations with particles in a frozen, kinematic velocity field showed that the subgrid scales reconstructed with the new model enhance mixing and result in improved profiles of particle properties as compared with reference data. In the following, basic assumption of the new approach are presented in more detail.

2 Fractal interpolation techniques with random stretching parameter

2.1 Basics

The fractal interpolation technique is an iterative procedure used to construct the synthetic velocity field of small-scale eddies $\mathbf{u}(\mathbf{x},t)$ from the knowledge of a filtered or coarse-grained field $\tilde{\mathbf{u}}(\mathbf{x},t)$ [28]. For this, the mapping operator, denoted by $W[.]$ is applied n times to $\tilde{\mathbf{u}}(\mathbf{x},t)$ to generate synthetic small scale velocity fields

$$\mathbf{u}_f(\mathbf{x},t) = W^{(n)}[\tilde{\mathbf{u}}(\mathbf{x},t)] \equiv W[W[W...W[\tilde{\mathbf{u}}(\mathbf{x},t)]...]].$$

As the turbulence energy spectrum has a high wavenumber cut-off set by the Kolmogorov scales, the limit $n \to \infty$ is not considered here. In practice, in order to stay at an acceptable numerical cost, the number of reconstruction steps is limited to 2 or 3. In the reconstruction process a crucial role is played by a prescribed stretching parameter d, which determines the amplitude and hence, the energy, of the reconstructed structures. For details of the procedure the reader is referred to [28].

Figure 1 shows the 1-D construction of a signal. To the initial field with three grid points we successively apply the map W with stretching parameter $d = \pm 2^{-1/3}$. Shown are the initial field, first, second, fourth and the tenth application of the map. With the chosen d the energy spectrum of the reconstructed signal generally follows the $-5/3$ profile observed in turbulence.

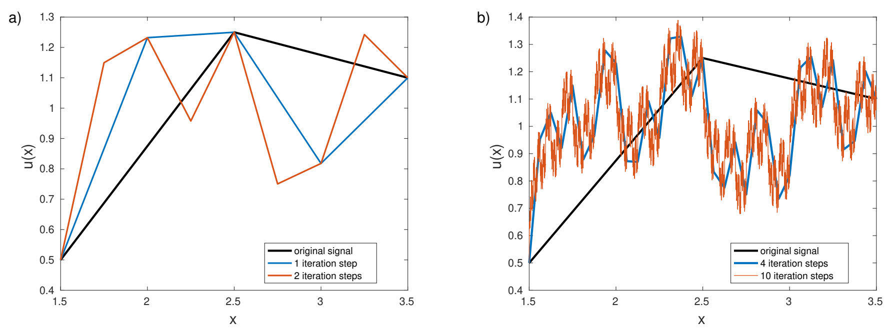

Figure 1: Different stages during the construction of a fractal function with stretching parameter $d = \pm 2^{-1/3}$ after (a) 0,1 and 2 reconstruction steps (b) 0, 4 and 10 reconstruction steps. Figure from Ref. [2].

2.2 Stretching parameter estimation

To estimate variability of d in turbulence we use an algorithm proposed by Mazel and Hayes [20]. Given velocity field specified on a grid, one value of d can be calculated for each set of 5 grid points. We applied this algorithm on a 1-D intersections of velocity field of a stratocumulus cloud. For this, we used three different datasets: DNS of stratocumulus-top boundary layer of [30] with relatively low Reynolds number, ($Re_\lambda = u'\lambda/\nu \approx 190$, where u' is the turbulence intensity, λ is the Taylor's microscale and ν is the kinematic viscosity of air), LES of stratocumulus top boundary layer of [23] with $Re_\lambda \approx 3900$ and, finally, experimental data of horizontal segments of flight 13 of the Physics of Stratocumulus Top (POST) research campaign [11, 15] with the same $Re_\lambda \approx 3900$.

Due to mathematical constrains the FIT reconstruction can be performed for d with values within the interval $(-1,1)$. In order to satisfy this condition, we placed a constraint $|d| \leq 1$ in the calculation of local stretching parameters and neglected d values outside this interval. In the case of DNS data described, we used horizontal profiles of the u, v and w components of velocity at a height corresponding to the in-cloud region.

1-D intersections of velocity field were filtered successively to wavenumber in the inertial range, starting from the initial resolution η_0, to $2\eta_0$ after one low-pass filtering, $4\eta_0$ after two filtering operations etc., until the resolution matched the inertial-range (at about $16\eta_0$ to $128\eta_0$). This was done with decimate function in MATLAB® software. The calculated PDFs changed significantly for the first four successive filtering steps but seemed to be self-similar when filtered successively to inertial-range wavenumbers (at steps 4 to 7). All three velocity components give similar profiles of the PDF of the stretching parameter. Next, PDF of d was calculated from LES field and from the POST airborne dataset using the same algorithm. In spite of different Re numbers we observe a very good agreement between the profiles as seen in Fig. 2. This results allows us to conclude that in the considered range of d, which is within the interval $(-1,1)$, the PDF of the stretching parameter in the inertial range is a universal function, independent of the Reynolds number. This fact is the basis of the model proposal described in the following subsection.

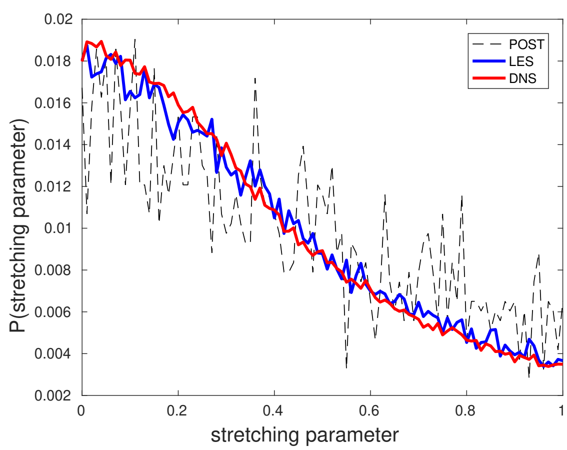

Figure 2: Probability distribution of stretching parameter from filtered DNS, LES velocity signals of stratocumulus cloud-top and POST data. DNS and LES velocity fields were filtered with wavenumber within the inertial range.

2.3 Fractal interpolation of filtered DNS

To reconstruct the signal we use the previously determined PDF profile, as shown in Fig. 2. For this we apply the inverse transform sampling method [8]. The algorithm is briefly indicated as follows

1. Calculate cumulative distribution function $F(|\mathrm{d}|)$ from the PDF $f(|\mathrm{d}|)$, as

$$F(|\mathrm{d}|) = \int_0^{|d|} f(s)ds.$$

2. Calculate the inverse of the cumulative function $F^{-1}(\mathrm{y})$.

3. Select a random number y from a uniform distribution $[0,1]$.

4. Calculate the random stretching coefficient as $d = F^{-1}(y)$, separately for each new grid point.

5. Reconstruct the signal by applying the mapping with random coefficients.

Apart from the mathematical constraint $|d| \leq 1$, which assures the continuity of the reconstructed signal at $n \to \infty$ reconstruction steps [5], the second constraint is related to the dissipative properties of the signal [27] and reads $|d| > 0.5$. Hence, in practice, in the reconstruction process we only retained the values $|d|$ that were larger than 0.5. If selected $|d| \leq 0.5$, the procedure was repeated and another random value was chosen, till the condition $0.5 < |d| \leq 1$ was satisfied. Next, the sign of d was selected randomly, such that the positive and negative d have equal probabilities.

Results of the reconstruction process were compared with results of the original model of Scotti & Meneveau [28], with $d = \pm 2^{1/3}$ and with the proposal of Basu et al. [6], where $d_1 = -0.887$, $d_2 = -0.676$. Figure 3 shows the frequency spectrum of a longitudinal velocity component measured in POST campaign with the spectrum of FIT-reconstructed velocity. As can be observed, the FIT energy spectrum reconstructed with random values of d follows the inertial-range scaling closer and shows no periodic modulation.

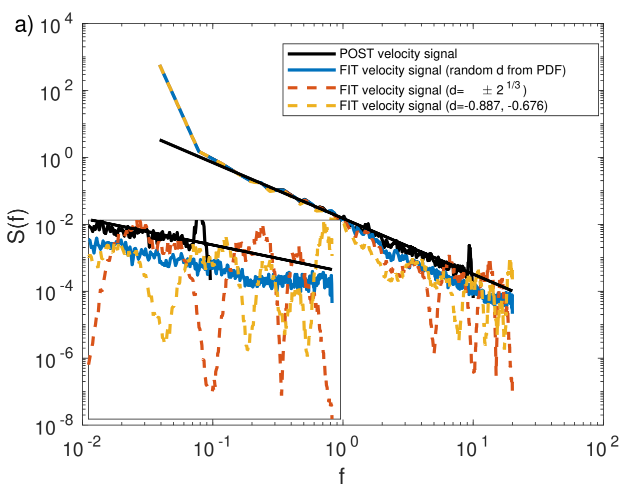

Figure 3: Longitudinal energy spectra of u velocity component for DNS and FIT with constant stretching parameter $d = \pm 2^{-1/3}$, with constant stretching parameters $d = -0.887$ and $d = -0.676$ and with random stretching parameters from calculated PDF. Figure from Ref. [2].

Next, statistics of velocity increments at two different points $\mathbf{u}(\mathbf{x}+\mathbf{r},t) - \mathbf{u}(\mathbf{x},t)$ were investigated. The non-Gaussianity of the PDFs of velocity increments for small distances $r = |\mathbf{r}|$ between the points indicates the presence of the internal intermittency, that is, the high probability of extreme events (large velocity differences). Reproducing this feature is important in modelling of interactions between particles (droplets) and turbulence. It was found from the analysis that results of all three FIT approaches compare well with the corresponding DNS profiles for large and intermediate values of r. However, with the decreasing distance r the new approach became clearly advantageous, see Fig. 4. For a more detailed description of analysis and results the reader is referred to [2].

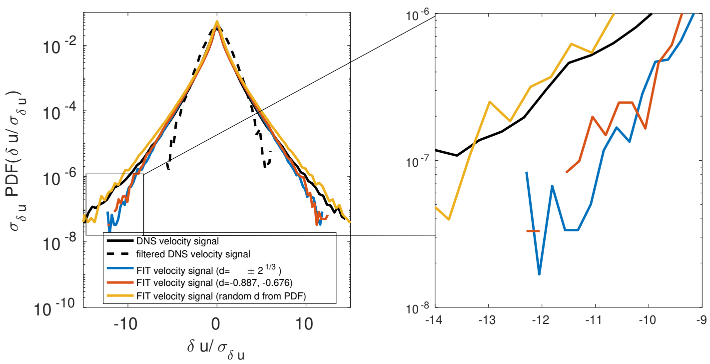

Figure 4: PDFs of velocity increments of DNS, filtered DNS and FIT fields at $|\mathbf{r}| = 2\eta_0$ with constant stretching parameter $d = \pm 2^{-1/3}$, $d = -0.887$ and $d = -0.676$ and random stretching parameters from PDF. Figure from Ref. [2].

2.4 Preliminary results for cloud droplets.

Shima et al. [29] proposed a Lagrangian technique for the simulation of cloud microphysics, named the super-droplet method. Each super-droplet for represents a multiplicity of real-world droplets with the same position, radius and composition. Two mutually coupled components form the framework for this method. These are the Eulerian fluid flow solver to calculate turbulent velocity field and a Lagrangian particle-tracking of physical coordinates and physicochemical properties of droplets in the turbulent flow. The condensation and evaporation of water on the super-droplets is represented as the source or sink of water vapour and heat, which the Eulerian component feeds on. The Lagrangian component needs the fluid velocity field in order to update both the positions of the super-droplets and the thermodynamic fields, which is needed to compute condensational growth and evaporation rates. The fractal subgrid scale model can also be used to account for the effect of the subgrid scales on super-droplet motion and growth/evaporation. As a preliminary test for the fractal sub-grid scale model, Lagrangian tracking of super-droplets in a frozen LES field of stratocumulus cloud [23] was performed. For simplicity, the super-droplets have only one attribute denoted as A_i. The computational domain is partitioned equally into two sub-domains in the x- direction. Super-droplets were initially positioned randomly within the domain. Droplets in the first half of domain had attribute $A_i = 0$ while the remaining ones were placed in the other half with attribute $A_i = 0$. The initial positions of droplets in x-, y- and z- directions were chosen randomly from the uniform distribution. A total of 300000 super-droplets were used for this analysis, such that on average, two super-droplets were placed in each LES computational cell. In this preliminary study droplets were treated as passive tracers and tracked in the velocity field of large eddies. After certain time their properties were averaged in the x and y directions. For the tracking of particles three different velocity fields were used: original LES field from Ref. [23], filtered LES after application of the decimate filter twice and finally, velocity field reconstructed back to the resolution of the original LES using the described FIT approach. Here, simulations with the original LES field will be treated as reference data. Low-pass filtering of some of the eddy structures results in reduced mixing and different evolution of the averaged particle properties. At the beginning of simulations all three profiles of averaged particle attributes are identical. Deviations between LES and filtered LES case are already visible after 30 *min* of simulation time, see Fig. 5a and grow in time, Fig. 5b. Due to the absence of smaller eddies in the velocity field the latter profile is sharper. It is also seen in Fig. 5 that the introduction of FIT-reconstructed scales enhances the mixing and improves the calculated statistics.

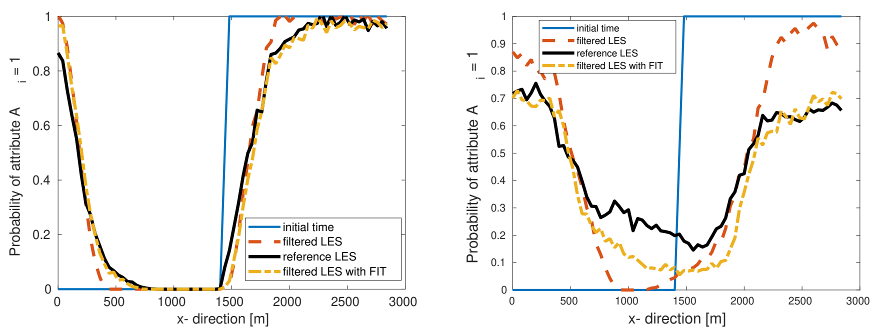

Figure 5: Averaged particle attribute in LES field of startocumulus cloud-top from Ref. [23] after simulation time a) 30 min, b) 2 hours.

Conclusions

The described new LES model conception on the interface/droplets interaction is related to the fractal interpolation technique. Based on analysis of numerical and experimental data it was found that for scales from the inertial range, the PDF of the stretching parameters is a universal function, independent of the Reynolds number. In the new approach we proposed to treat the stretching parameter of the FIT as a random function with the prescribed PDF. As it was found, the new approach results in improved statistics of the subgrid scales. Preliminary results with droplets' simulations in a frozen kinematic field prove that FIT reconstruction of the subfilter eddies enhances the mixing and improves calculated statistics of particle attributes.

With this the model is ready to be applied to full large eddy simulation coupled with the super-droplet approach of [29] to account for the effect of the subgrid scales on super-droplet motion and growth/evaporation on the cloud/clear-air interface.

References

[1] Akinlabi E. O., Wacławczyk M., Malinowski S. P.: Fractal reconstruction of sub-grid scales for large eddy simulation of atmospheric turbulence, J. Phys.: Conf. Ser., 1101, 012001 (2018) `doi:10.1088/1742-6596/1101/1/0120012018`

[2] Akinlabi, E.O., Wacławczyk M., Malinowski, S.P., Mellado J. P.: Fractal Reconstruction of Sub-Grid Scales for Large Eddy Simulation. Flow Turbulence Combust 103, 293 (2019)

Akinlabi E. O., Wacławczyk M., Malinowski S. P.: Fractal reconstruction of sub-grid scales for large eddy simulation of atmospheric turbulence, J. Phys.: Conf. Ser., 1101, 012001 (2018) `doi:10.1088/1742-6596/1101/1/0120012018`

[3] Andrejczuk M., Grabowski W. W., Malinowski S. P., Smolarkiewicz P. K.: Numerical simulation of cloudclear air interfacial mixing. Journal of the Atmospheric Sciences, 61(14), 17261739 (2004)

[4] Arabas S. and Shima S.: Large-Eddy Simulations of Trade Wind Cumuli Using Particle-Based Microphysics with Monte Carlo Coalescence, J. Atmos. Sci., 70, 27682777 (2013) `https://doi.org/10.1175/JAS-D-12-0295.1`

[5] Barnley M.F: Constructive Approximation 2, 303-329 (1986).

[6] Basu S., Foufoula-Georgiou E., Porte-Agel F.: Synthetic Turbulence, Fractal interpolation and Large Eddy Simulation, Phys. Rev. E70, 026310, (2004)

[7] Das S. K. and Durbin P. A.: A Lagrangian stochastic model for dispersion in stratified turbulence, Phys. Fluids, 17, 025109 (2005)

[8] Devroye L.: Non-uniform random variate generation, Springer-Verlag New York Inc. (1986)

[9] Dziekan P. and Pawlowska H.: Stochastic coalescence in Lagrangian cloud microphysics, Atmos. Chem. Phys., 17, 13509-13520 (2017) `https://doi.org/10.5194/acp-17-13509-2017`

[10] Fung J. C. H., Vassilicos J. C.: Two-particle dispersion in turbulentlike flows, Phys. Rev. E, 57, 1677-1690 (1998)

[11] Gerber H, Frick G, Malinowski S P, Jonsson H, Khelif D and Krueger S K.: Entrainment rates and microphysics in POST stratocumulus J. Geophys. Res. Atmos. 118 (2013) (`https://doi:10.1002/jgrd.50878`)

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[12] Geurts B. J.: Inverse modeling for large eddy simulation, Phys. Fluids 9, 3585 (1997)

[13] Gobert C. and Manhart M.: Subgrid modeling for particle-LES by spectrally optimized interpolation (SOI), J. Comput. Phys., 230, 7796-7820, (2011)

[14] Grabowski W. W.: Indirect impact of atmospheric aerosols inidealized simulations of convectiveradiative quasi-equilibrium, J. Climate, 19, 46644682 (2006)

[15] Jen-La Plante I., Ma Y., Nurowska K., Gerber H., Khelif D., Karpinska K., Kopec M. K., Kumala W, Malinowski S. P.: Physics of Stratocumulus Top (POST): turbulence characteristics, Atmos. Chem. Phys., 16(15), 9711-9725, (2016)

[16] Kumar, B., Götzfried, P., Suresh, N., Schumacher, J., Shaw, R. A.: Scale dependence of cloud microphysical response to turbulent entrainment and mixing. Journal of Advances in Modeling Earth Systems, 10, 2777 2785, (2018)

[17] Malinowski S. P., Zawadzki I.: On the Surface of Clouds, Journal of the Atmospheric Sciences, 50 , 5-13 (1993)

[18] Marchioli C., Salvetti M.V., Soldati A.: Appraisal of energy recovering sub-grid scale models for large eddy simulation of turbulent dispersed flows, Acta Mech, 201, 277-296 (2008)

[19] Marchioli C.: Large-eddy simulation of turbulent dispersed flows: a review of modelling approaches, Acta Mech, 228:741 (2017) `https://doi.org/10.1007/s00707-017-1803-x`

[20] Mazel D. S., Hayes M. H.: Using Iterated Function systems to model discrete sequences, IEEE Trans. on signal processing, 40(7), (1992)

[21] Mellado J. P.: Cloud-top entrainment in stratocumulus clouds, Annu. Rev. Fluid Mech., 49, 145-169, (2017)

[22] Minier J-P, Pozorski J.: Particles in Wall-Bounded Turbulent Flows: Deposition, Re-Suspension and Agglomeration, Springer, 571, 0254-1971, (2017). `doi:10.1007/978-3-319-41567-3`

[23] Pedersen J. G., Ma Y.F., Grabowski W. W., Malinowski, S. P.: Anisotropy of observed and simulated turbulence in marine stratocumulus. J. Adv. Model. Earth Syst., 10, 500515 (2018)

[24] Pope S. B.: Turbulent Flows, Cambridge University Press, Cambridge, (2000)

[25] Pozorski J., Apte S. V.: Filtered particle tracking in isotropic turbulence and stochastic modeling of sub-grid scale dispersion, Int. J. Multiphase Flow, 35, 118-128 (2009)

[26] Pozorski J., Rosa B.: The motion of settling particles in isotropic turbulence: filtering impact and kinematic simulations as subfilter model, Direct and Large Eddy Simulation XI, 6 pp. Springer, *in press* (2018)

[27] Scotti A., Meneveau C. and Saddoughi S.G.: Fractal dimension of velocity signals in high Reynolds number hydrodynamic turbulence, Phys. Rev. E 51, 5594 - 5608, (1995)

[28] Scotti A., Meneveau C.: A fractal model for large eddy simulation of turbulent flow, Physica D, 127 198232, (1999)

[29] Shima S., Kusano K., Kawano A., Sugiyama T. and Kawahara S.: The super-droplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model, Q. J. R. Meteorol. Soc., 135, 13071320 (2009)

[30] Schulz B. and Mellado J.P.: Wind Shear Effects on Radiatively and Evaporatively Driven Stratocumulus Tops, J. Atmos. Sci., 75, 32453263 (2018) https://doi.org/10.1175/JAS-D-18-0027.1

[31] Stolz S., Adams N. A. and Kleiser L.: An approximate deconvolution model for large eddy simulation with application to incompressible wall-bounded flows, Phys. Fluids, 13, 997 (2001)