Implementation of TKE–Scalar Variance Mixing Scheme into COSMO

Ekaterina Machulskaya and Dmitrii Mironov

German Weather Service, Offenbach am Main, Germany

1 Introduction

We report on the development and testing of a turbulence kinetic energy – scalar variance (TKESV) mixing scheme, and its implementation into the COSMO model. A summary of results obtained within the framework of the COSMO Priority Project UTCS is given, including a brief outline of the TKESV scheme, a discussion of the scheme performance in various clear and cloudy boundary-layer regimes as revealed by off-line single-column tests, details of the implementation of the new scheme into COSMO, and some results from numerical experiments with the full-fledged COSMO model. Future challenges are briefly discussed.

In what follows, standard notation is used, where t is the time, x_i are the space co-ordinates, and u_i are the velocity components (the subscript "3" refers to the vertical direction). The angle brackets denote a (grid-box) mean quantity, and a prime denotes a fluctuation about the mean.

2 Outline of the TKESV scheme

A turbulence kinetic energy – scalar variance mixing scheme for the COSMO model is developed. The scheme is formulated in terms of two scalars that are approximately conserved for phase changes in the absence of precipitation. These are the total water specific humidity q_t and the liquid water potential temperature θ_l. The TKESV scheme carries prognostic transport equations for the turbulence kinetic energy (TKE), $\frac{1}{2}\left\langle u_i'^2\right\rangle$, for the variances of the scalar quantities, $\left\langle q_t'^2\right\rangle$ and $\left\langle \theta_l'^2\right\rangle$, and for their covariance, $\langle q_t'\theta_l'\rangle$. The other second-order moments, viz., the Reynolds stress, $\left\langle u_i'u_j'\right\rangle$, and the scalar fluxes, $\langle u_i'q_t'\rangle$ and $\langle u_i'\theta_l'\rangle$, are determined through the algebraic diagnostic expressions obtained by neglecting the time-rate-of-change and the triple correlations terms in the respective transport equations. Notice that $\left\langle q_t'^2\right\rangle$, $\left\langle \theta_l'^2\right\rangle$ and $\langle q_t'\theta_l'\rangle$ actually characterize the potential energy of fluctuating fields, i.e. the turbulence potential energy.

A one-dimensional transport equation for the covariance of two generic scalars a and b reads

$$\frac{\partial \langle a'b'\rangle}{\partial t} = -\left\langle u_3'a'\right\rangle \frac{\partial \langle b\rangle}{\partial x_3} - \left\langle u_3'b'\right\rangle \frac{\partial \langle a\rangle}{\partial x_3} - \frac{\partial}{\partial x_3}\left\langle u_3'a'b'\right\rangle - \epsilon_{ab}, \tag{1}$$

where $\epsilon_{ab} = (\kappa_a + \kappa_b)\left\langle \frac{\partial a'}{\partial x_i}\frac{\partial b'}{\partial x_i}\right\rangle$ is the molecular destruction (dissipation) rate of the co-variance $\langle a'b'\rangle$, and κ_a and κ_b are the molecular diffusivities for the quantities a and b, respectively. The transport equations for the variances of q_t and θ_l and for their covariance are obtained from Eq. (1) by setting $a = b = q_t$, $a = b = \theta_l$, and $a = q_t$ and $b = \theta_l$, respectively.

The turbulent transport terms in the scalar (co-)variance equations, i.e. the divergence of the velocity-scalar triple correlations as given by the third term on the right-hand side of Eq. (1), are parameterized through advanced "diffusion+advection" formulations that account for the skewed nature of convective motions [12]. The scalar skewness is obtained from its own transport equation where closure assumptions for the unknown terms are formulated with due regard for non-Gaussianity of fluctuating fields [5, 6]. The turbulent transport term in the TKE equation (the divergence of the velocity-velocity triple correlation and the pressure-velocity correlation) is parameterized through a down-gradient diffusion formulation. The pressure scrambling terms in the Reynolds-stress and scalar-flux equations are parameterized with due regard for turbulence anisotropy. The dissipation terms in the TKE and in the scalar (co-)variance equations are parameterized through relaxation approximations in terms of dissipation time scales. The various time scales, viz., the dissipation time scales in the TKE and scalar (co)-variance equations and the return-to-isotropy time scales in the Reynolds-stress and scalar-flux equations, are set proportional to each other and are expressed in terms of turbulence length scale and the TKE. The formulation for the turbulence length scale accounts for the effect of static stability. A statistical cloud scheme is used to parameterize the effect of sub-grid scale (SGS) condensation (cloudiness) on the buoyancy production of TKE. A Gaussian scheme [20] modified to account, in a very approximate way, for the skewness of temperature and humidity fields [2] is utilized.

A detailed description of the TKESV scheme will be given in subsequent publications. An extended discussion of turbulence parameterization schemes used in numerical models of the atmosphere is given in [11].

It should be emphasized that within the framework of the current COSMO-model turbulence scheme [17, 18, 1], the time-rate-of-change and the turbulent transport terms are retained in the TKE equation only, whereas all other second-order moments, including scalar (co-)variances, are determined from the algebraic diagnostic expressions. As a consequence, the expressions for the scalar fluxes do not include non-gradient terms and do not allow for up-gradient heat transfer that is known to occur in many convective flows, e.g. in the cloud-free convective planetary boundary layer (PBL) or in the sub-cloud layer of cloud-topped PBLs. This can be readily verified by neglecting the left-hand side and the third term on the right-hand side of Eq. (1) and setting $a = b = \theta$, where θ is the potential temperature (θ_l is equal to θ if clouds are absent). Then, $-\langle u_3'\theta'\rangle\, \partial\langle\theta\rangle/\partial x_3 - \epsilon_{\theta\theta} = 0$, indicating that the up-gradient hear transfer, when the temperature flux $\langle u_3'\theta'\rangle$ and the temperature gradient $\partial\langle\theta\rangle/\partial x_3$ have the same sign, would mean physically impossible negative temperature-variance dissipation rate. It should also be noted that the current COSMO-model turbulence scheme utilizes a Blackadar-type turbulence length scale formulation independent of static stability and a quasi-Gaussian statistical cloud scheme (see [1] for details).

3 Single-column tests

The TKESV scheme is tested through a series of single-column numerical experiments. Results from experiments with the TKESV and the TKE schemes are compared with observational and numerical large-eddy simulation (LES) data from dry convective PBL and from cloudy PBLs (BOMEX and ARM shallow cumulus cases and DYCOMS-II stratocumulus case).

Figure 1 shows vertical profiles of potential temperature in the shear-free dry convective PBL driven by the surface buoyancy flux. As revealed by comparison of model results with the LES data from [13], the TKESV scheme clearly outperforms the TKE scheme. A well-mixed character of (the bulk of) dry convective PBL and up-gradient heat transfer in the upper part of the mixed layer, where the potential-temperature gradient and the heat flux are both positive, are well reproduced by the TKESV scheme. The TKE scheme gives an excessive (negative) potential-temperature gradient in most of the PBL and is incapable of reproducing up-gradient heat transfer due to the use of down-gradient formulations for the scalar fluxes. In Fig. 2, vertical profiles of the TKE and of the potential-temperature variance computed with the TKESV and the TKE schemes are compared with the LES data. Results from numerical experiments with the TKESV scheme are in better agreement with data, although both schemes invite further improvements. Note that the TKE scheme yields zero potential-temperature variance in the upper part of the mixed layer where the temperature gradient changes sign. This result is spurious. It stems from the neglect of the third-order transport (diffusion) of scalar variances within the TKE scheme, where the scalar-variance equations are reduced (truncated) to the balance between the mean-gradient production and dissipation. The TKESV scheme does account for the third-order transport of scalar variances and yields better estimates of the variances throughout the convective PBL.

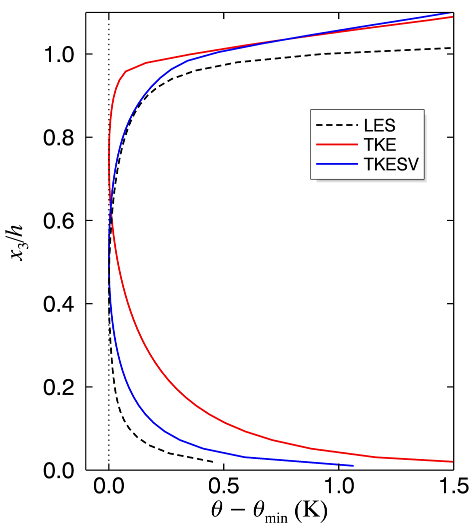

Figure 1: Potential temperature minus its minimum value vs. dimensionless height (h is the PBL depth) in the dry convective PBL. Black dashed curve shows LES data [13], and solid curves show results from numerical experiments with the TKE (red) and TKESV (blue) schemes.

The application of the TKESV and TKE scheme to the stratocumulus-topped PBL (DYCOMS-II test case, see [21]) reveal a similar performance of the two schemes. The TKESV scheme brings about minor improvements as to the scalar variances $\langle \theta_l'^2 \rangle$ and $\langle q_t'^2 \rangle$. In the shallow-cumulus regime (BOMEX test case, see [9, 19]), the application of the TKESV scheme leads to a better prediction of the scalar variances (Fig. 3), and to slight improvements with respect to the TKE, the vertical buoyancy flux and the mean temperature and humidity. A detailed analysis of results from numerical experiments suggests that the major difficulties in modelling the shallow cumulus regime are associated with the representation of the fractional cloud cover and its effect on the buoyancy flux. A quasi-Gaussian cloud parameterization used operationally in the COSMO model strongly overestimates fractional cloud cover in the cumulus-topped PBL. A modified parameterization with an ad hoc non-Gaussian correction [2] improves the fractional cloud cover. Both cloud parameterizations fail to accurately describe the effect of fractional cloudiness on the buoyancy flux (buoyancy production of TKE) in the shallow cumulus regime (although the parameterization with non-Gaussian correction does a slightly better job). A somewhat more sophisticated cloud scheme that accounts for non-Gaussian effects (e.g. through the skewness of scalar fields) is required.

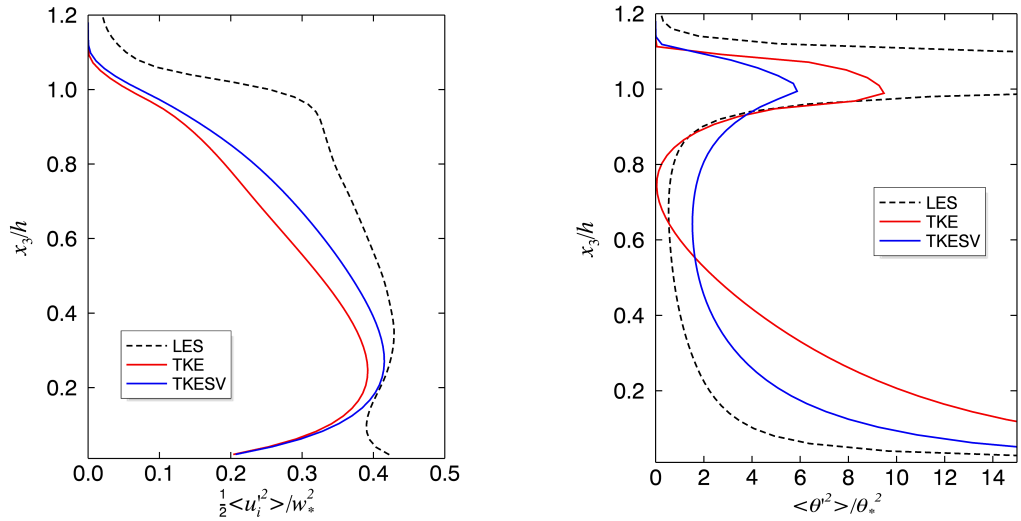

Figure 2: TKE (left panel) and potential temperature variance (right panel) vs. dimensionless height (h is the PBL depth) in the dry convective PBL. Black dashed curves show LES data [13], and solid curves show results from numerical experiments with the TKE (red) and TKESV (blue) schemes. Profiles are made dimensionless with the Deardorff [3, 4] convective scales of velocity, w_*, and temperature, θ_*.

4 Implementation into COSMO model

The TKESV scheme is implemented into the COSMO model and tested through a series of parallel experiments including the entire COSMO-model data assimilation cycle. Both COSMO-EU and COSMO-DE model configurations operational at DWD are used. The horizontal mesh size of these configurations is ca. 7 km and ca. 2.8 km, respectively. In the parallel experiments, the skewness-dependent "diffusion+advection" parameterizations of the third-order moments in the scalar (co-)variance equations are not used; instead, the third-order moments (fluxes of (co-)variances) are determined through the down-gradient formulations. Although the diffusion+advection parameterizations are available as an option, they are not recommended for immediate use with the full-fledged COSMO model. The use of the skewness-dependent third-order moments reduces numerical stability of the entire scheme. Then, a smaller time step is required, making the scheme computationally too expensive for current operational applications.

Results from the COSMO-EU and COSMO-DE parallel experiments with the TKESV scheme performed to date look promising. Verification of results against observational data indicate perceptible improvements as to some scores, e.g. two-metre temperature and humidity. Verification results show marginal improvements with respect to fractional cloud cover and no detectable changes with respect to precipitation. Performance of the TKESV scheme is exemplified by Figs. 4 and 5. The use of the TKESV scheme within COSMO-DE leads to a noticeable reduction of both bias and root-mean-square error (RMSE) of two-metre temperature and dew point depression. It should be emphasized that the curves in Figs. 4 and 5 are the result of averaging over the entire COSMO-DE domain. Local positive effects of the TKESV scheme on the COSMO-DE performance are often more pronounced.

As the results from the LES study of Mironov and Sullivan [16] demonstrate, the stably stratified PBL should be parameterized with due regard for the SGS heterogeneity of the

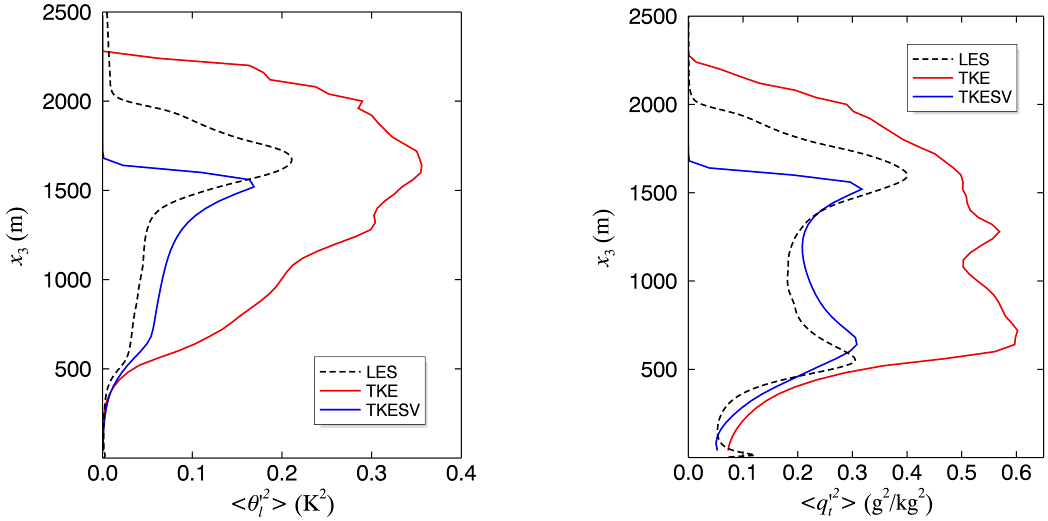

Figure 3: Variances of the liquid water potential temperature (left panel) and of the total water specific humidity (right panel) in the shallow-cumulus-topped PBL. Black dashed curves show data from LES of BOMEX shallow cumulus case performed by Heinze [7], and solid curves show results from numerical experiments with the TKE (red) and TKESV (blue) schemes. Both schemes use the cloud parameterization proposed in [2].

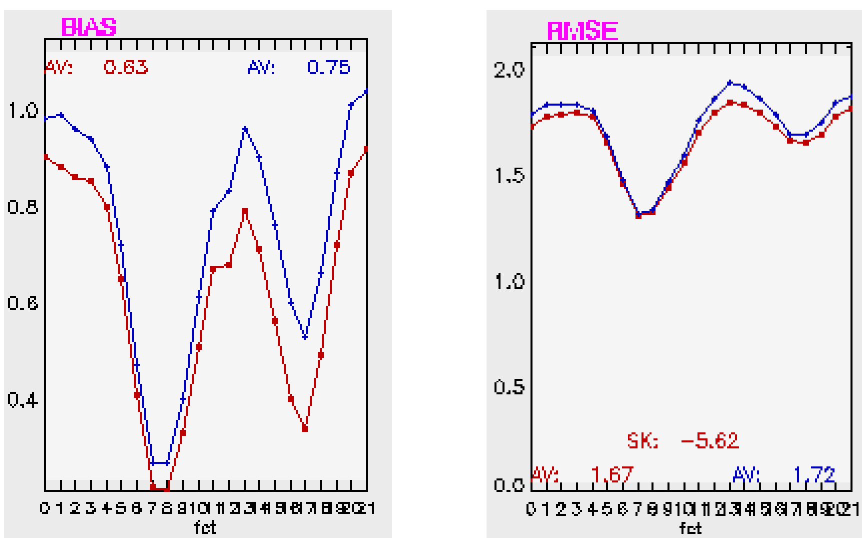

Figure 4: Bias (left panel) and RMSE (right panel) of two-metre temperature over the period from 1 July 2011 through 30 September 2011. Blue curves show operational COSMO-DE results, and red curves show results from parallel experiment with the new TKESV scheme. The curves are obtained by means of averaging over the COSMO-DE domain.

underlying surface, first of all, with respect to the temperature. An LES-based analysis of the second-moment budgets shows that the enhanced mixing in the heterogeneous stably stratified PBL is mainly due to a strong increase of the temperature variance near the underlying surface and the ensuing decrease of the magnitude of the (negative) buoyancy flux (cf. the importance of scalar variances in convective PBLs). As discussed in [16], there are

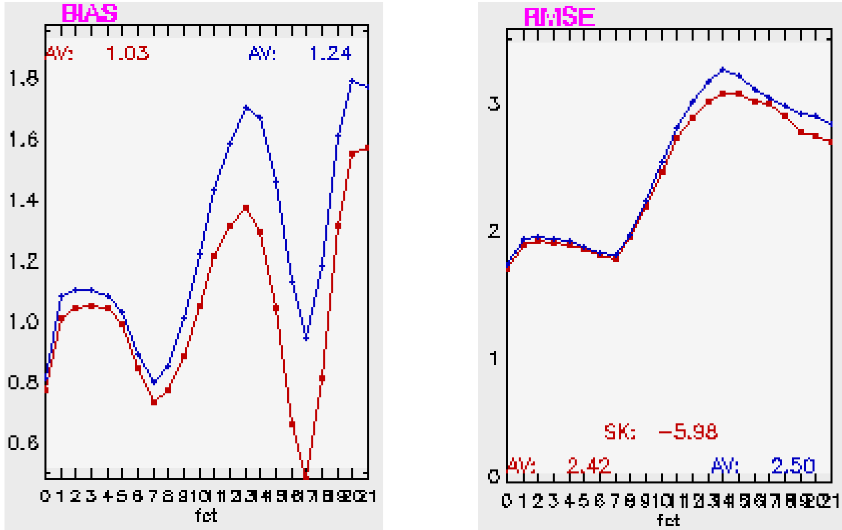

Figure 5: The same as in Fig. 4 but for the two-metre dew point depression.

several conceivable ways to account for this effect. One feasible way is the application of a tile approach. It allows to account for the enhanced mixing over heterogeneous surfaces in a physically plausible way and to prevent the PBL turbulence from dying out entirely as the (grid-box mean) static stability increases[1]. The idea is successfully tested through single-column numerical experiments (e.g. the increase of temperature variance and the enhancement of mixing over heterogeneous surfaces are reproduced). The number of tiles should not necessarily be large (otherwise the tiled scheme becomes computationally expensive) but the tiles with the largest difference in terms of thermal inertia should be accounted for. In this regard, the treatment of SGS water bodies is crucial. As the thermal inertia of water is (much) larger than the inertia of most other land types, the inclusion of SGS water allows to maintain the temperature difference between tiles and hence to account for the enhanced mixing due to surface heterogeneity. A parallel COSMO-EU experiment with a "two-tile" surface scheme is performed, where a "land tile" with the land-use type the same as in the operational COSMO model and an "inland water tile" ("lake") are considered in each COSMO-model grid box. The surface temperature of the inland water tile is computed with the lake parameterization scheme FLake [10, 14, 15]. Recall that in the operational COSMO configurations, only the grid boxes with the inland water fraction in excess of 0.5 are treated as the inland-water-type grid boxes whereas the SGS water bodies with fractional area coverage less than 0.5 are entirely ignored. Results from the parallel experiment indicate some improvements of the COSMO-model performance, e.g. warm bias of the near-surface temperature during summer is reduced.

[1]Cf. a long-standing COSMO-model problem with too large minimum diffusion coefficients that are used as a (unphysical) proxy for unaccounted mixing processes. These "background" diffusivities are insensitive to the mixing regime. They prevent the collapse of mixing but are often detrimental for stably stratified PBLs and for the inversions capping convective PBLs (produce too strong mixing where it is not needed). On the contrary, the TKESV scheme coupled to a tiled surface scheme is selective in terms of mixing regimes. For example, it produces enhanced mixing in the core of convective PBL but does not mix too strongly in the upper part of the stably stratified PBL and in the capping inversion.

5 Summary and outlook

A turbulence kinetic energy – scalar variance mixing scheme for COSMO is developed and favourably tested through single-column numerical experiments and through parallel experiments with the full-fledged COSMO model including the entire data assimilation cycle. The TKESV scheme outperforms the current COSMO-model TKE scheme. Verification of results from parallel experiments indicate improvements as to some scores, e.g. two-metre temperature and humidity and fractional cloud cover. A detailed scientific documentation of the TKESV scheme is in preparation. Modifications associated with the TKESV scheme will soon be included into the official COSMO-model code (for details, see the Priority Project UTCS Reports and the Model Development Plan at the COSMO web site).

In the future, the following issues should be addressed to further improve the COSMO-model mixing scheme.

(i) Development of a three-moment (mean, variance, and skewness) statistical cloud scheme capable of predicting the fractional cloud cover and the buoyancy flux in cloudy PBLs with due regard for non-Gaussian effects. This work is carried out by A. Seifert and A.-K. Naumann within the framework of the Hans Ertel Centre on Cloud and Convection, Hamburg. The major part of the work is completed (Naumann, A.-K., A. Seifert, and J. P. Mellado, 2013: A refined statistical cloud closure using double-Gaussian probability density functions. Submitted to *Geosci. Model Dev.*).

(ii) Further development and comprehensive testing of transport equations for the skewness of scalar quantities, coupling the skewness equations with the three-moment statistical cloud scheme. Closure assumptions for the scalar skewness equations and a skewness-dependent "diffusion+advection" parameterizations of the third-order moments in the scalar variance equations are developed and tested through single-column numerical experiments. They are available as an option within the TKESV scheme. These parameterizations are, however, not recommended for the immediate implementation into COSMO due to numerical stability problems (a smaller time step is required). The skewness-dependent parameterizations of the third-order transport may be used in the future, but further analysis, testing and tuning are required. However, the scalar skewness equations decoupled from the third-order transport but coupled to the statistical cloud scheme is a viable next-step option.

(iii) Improved coupling of the scalar (co-)variance equations to the tiled surface scheme to better account for the effect of surface heterogeneity on the structure and mixing properties of the PBL (mainly the stably stratified PBL). To this end, effort should go into the analysis of various flow regimes over heterogeneous surfaces (e.g. temperature-heterogeneous flat surface versus temperature-homogeneous surface with orographic features such as hills and valleys) and of the surface boundary conditions for the scalar (co-)variances with due regard for the surface heterogeneity. This work is to a large extent based on the LES findings reported in [16]. Further results are expected from co-operative work with P. Sullivan of NCAR.

The LES data set [8, 7], developed at the University of Hannover by R. Heinze and S. Raasch within the framework of the "Extramurale Forschung" program of the German Weather Service and the German Universities, will be extensively used to tackle the above issues.

Acknowledgments. The authors are grateful to Euripides Avgoustoglou, Peter Bechtold, Vittorio Canuto, George Craig, Ulrich Damrath, Sergey Danilov, Evgeni Fedorovich, Jochen Förstner, Jean-Francois Geleyn, Federico Grazzini, Vladimir Gryanik, Thomas Hanisch, Rieke Heinze, Richard Keane, Friedrich Kupka, Donald Lenschow, Chin-Hoh Moeng, Ned Patton, Robert Plant, Siegfried Raasch, Matthias Raschendorfer, Bodo Ritter, Harald Ruppert, Ulrich Schättler, Balázs Szintai, Axel Seifert, Pier Siebesma, Alan Shapiro, Peter Sullivan, Jeffrey Weil, and Jun-Ichi Yano for discussions and helpful suggestions. Thanks are due to Rieke Heinze for providing LES data shown in Fig. 3.

References

[1] Baldauf, M., A. Seifert, J. Förstner, D. Majewski, M. Raschendorfer, and T. Reinhardt, 2001: Operational convective-scale numerical weather prediction with the COSMO model: description and sensitivities. *Mon. Weather Rev.*, **139**, 3887–3905.

[2] Bechtold, P., J. W. M. Cuijpers, P. Mascart, and P. Trouilhet, 1995: Modeling of trade wind cumuli with a low-order turbulence model: Toward a unified description of Cu and Sc clouds in meteorological models. *J. Atmos. Sci.*, **52**, 455–463.

[3] Deardorff, J. W., 1970: Preliminary results from numerical integrations of the unstable planetary boundary layer. *J. Atmos. Sci.*, **27**, 1209–1211.

[4] Deardorff, J. W., 1970: Convective velocity and temperature scales for the unstable planetary boundary layer and for Rayleigh convection. *J. Atmos. Sci.*, **27**, 1211–1213.

[5] Gryanik, V. M., and J. Hartmann, 2002: A turbulence closure for the convective boundary layer based on a two-scale mass-flux approach. *J. Atmos. Sci.*, **59**, 2729–2744.

[6] Gryanik, V. M., J. Hartmann, S. Raasch, and M. Schröter, 2005: A refinement of the Millionshchikov quasi-normality hypothesis for convective boundary layer turbulence. *J. Atmos. Sci.*, **62**, 2632–2638.

[7] Heinze, R., 2013: *Large-Eddy Simulation von bewölkten Grenzschichten zur Untersuchung von Bilanzen der statistischen Momente zweiter Ordnung und zur Überprüfung von Turbulenzmodellen.* PhD thesis, Der Fakultät für Mathematik und Physik der Gottfried Wilhelm Leibniz Universität Hannover, 153 pp.

[8] Heinze, R., D. Mironov, and S. Raasch, 2012: Budgets of scalar fluxes for cloudy boundary layers. *20th Amer. Meteorol. Soc. Symp. on Boundary Layers and Turbulence*, Boston, MA, USA, paper 11.4, 9 pp.

[9] Holland, J. Z., and E. M. Rasmusson, 1973: Measurements of the atmospheric mass, energy, and momentum budgets over a 500-kilometer square of tropical ocean. *Mon. Weather Rev.*, **101**, 44–55.

[10] Mironov, D., V., 2008: Parameterization of lakes in numerical weather prediction. Description of a lake model. *COSMO Technical Report*, No. 11, 41 pp.

[11] Mironov, D. V., 2009: Turbulence in the lower troposphere: second-order closure and mass-flux modelling frameworks. *Interdisciplinary Aspects of Turbulence*, Lect. Notes Phys., **756**, W. Hillebrandt and F. Kupka, Eds., Springer-Verlag, Berlin, Heidelberg, 161–221.

[12] Mironov, D. V., V. M. Gryanik, V. N. Lykossov, and S. S. Zilitinkevich, 1999: Comments on "A New Second-Order Turbulence Closure Scheme for the Planetary Boundary Layer" by K. Abdella and N. McFarlane. *J. Atmos. Sci.*, **56**, 3478–3481.

[13] Mironov, D., V., V. M. Gryanik, C.-H. Moeng, D. J. Olbers, and T. H. Warncke, 2000: Vertical turbulence structure and second-moment budgets in convection with rotation: a large-eddy simulation study. *Quart. J. Roy. Meteorol. Soc.*, **126**, 477–515.

[14] Mironov, D., E. Heise, E. Kourzeneva, B. Ritter, N. Schneider, and A. Terzhevik, 2010: Implementation of the lake parameterisation scheme FLake into the numerical weather prediction model COSMO. *Boreal Env. Res.*, **15**, 218–230.

[15] Mironov, D., B. Ritter, J.-P. Schulz, M. Buchhold, M. Lange, and E. Machulskaya, 2012: Parameterization of sea and lake ice in numerical weather prediction models of the German Weather Service. *Tellus A*, **64**, 17330. doi: 10.3402/tellusa.v64i0.17330

[16] Mironov, D. V., and P. P. Sullivan, 2010: Effect of horizontal surface temperature heterogeneity on turbulent mixing in the stably stratified atmospheric boundary layer. *19th Amer. Meteorol. Soc. Symp. on Boundary Layers and Turbulence*, Keystone, CO, USA, paper 6.3, 10 pp.

[17] Raschendorfer, M., 1999: Special topic: The new turbulence parameterization of LM. *Quarterly Report of the Operational NWP-Models of the Deutscher Wetterdienst*, No. 19, 3–12.

[18] Raschendorfer, M., 2001: The new turbulence parameterization of LM. *COSMO Newsletter*, No. 1 , 89–97.

[19] Siebesma, A. P., Ch. S. Bretherton, A. Brown, A. Chlond, J. Cuxart, P. G. Duynkerke, H. Jiang, M. Khairoutdinov, D. Lewellen, Ch.-H. Moeng, E. Sanchez, B. Stevens, and D. E. Stevens, 2003: A large eddy simulation intercomparison study of shallow cumulus convection. *J. Atmos. Sci.*, **60**, 1201–1219.

[20] Sommeria, G., and J. W. Deardorff, 1977: Subgrid-scale condensation in models of nonprecipitating clouds. *J. Atmos. Sci.*, **34**, 344–355.

[21] Stevens, B., C.-H. Moeng, A. S. Ackerman, Ch. S. Bretherton, A. Chlond, S. de Roode, J. Edwards, J.-Ch. Golaz, H. Jiang, M. Khairoutdinov, M. P. Kirkpatrick, D. C. Lewellen, A. Lock, F. Muller, D. E. Stevens, E. Whelan, and P. Zhud, 2005: Evaluation of large-eddy simulations via observations of nocturnal marine stratocumuls. *Mon. Weather Rev.*, **133**, 1443–1462.