

#### Implementation of a TKE-Scalar Variance Mixing Scheme into the COSMO Model

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## Outline



#### ➔ Motivation

- → Formulation of the TKE-Scalar Variance scheme
  - prognostic equations for scalar variances
  - non-local, skewed nature of convective motions
  - turbulence anisotropy
  - coupling with statistical cloud scheme
- → Single-column tests
- → Implementation into the COSMO model
- → Future challenges



### Motivation

Quoting Arakawa (2004, The Cumulus Parameterization Problem: Past, Present, and Future. *J. Climate*, **17**, 2493-2525), where, among other things,

"Major practical and conceptual problems in the conventional approach of cumulus parameterization, which include artificial separations of processes and scales, are discussed."

"It is rather obvious that for future climate models the scope of the problem must be drastically expanded from "cumulus parameterization" to "unified cloud parameterization" or even to "unified model physics". This is an extremely challenging task, both intellectually and computationally, and the use of multiple approaches is crucial even for a moderate success."

### Motivation (cont'd)

The tasks of developing a "unified cloud parameterization" and eventually a "unified model physics" seem to be too ambitious, at least at the moment.

# However, a unified description of turbulence and boundary-layer convection seems to be feasible.

There are several ways to do so (see Mironov 2009, for a detailed discussion). A viable option for high-resolution NWP is a non-local mixing scheme incl. mass-flux parameterization ideas "translated" into the language of second-order closures (see DM, EM & P. Sullivan presentation at the 8th SRNWP Workshop, Bad Orb, 2009).

### **TKE-Scalar Variance (TKESV) Scheme**

#### Key features

- prognostic treatment of TKE and of scalar variances with due regard for the third-order transport (+ diagnostic relations for scalar fluxes and Reynolds stress)
- account for non-local, skewed nature of convective motions
- account for turbulence anisotropy (via advanced parameterizations of pressure scrambling effects)
- intimate coupling with statistical cloud scheme

#### **TKE and Scalar Variances Have Equal Rights**

<u>Prognostic equations</u> for  $\langle u_i \rangle^2 \rangle$  (kinetic energy of SGS motions) and for  $\langle \theta_l \rangle^2 \rangle$ ,  $\langle q_t \rangle^2 \rangle$ ,  $\langle q_t \rangle^2 \rangle$  (potential energy of SGS motions) <u>including third-order transport</u>

Convection/stable stratification = Potential Energy ↔ Kinetic Energy **No reason to prefer one form of energy over the other!** 

A scalar-variance equation

$$\frac{1}{2} \frac{\partial \overline{\theta'}^2}{\partial t} = -\overline{w'\theta'} \frac{\partial \overline{\theta}}{\partial z} - \frac{1}{2} \frac{\partial}{\partial z} \overline{w'\theta'}^2 - \varepsilon_{\theta}$$
non-stationarity non-homogeneity

<u>Terms underlined red are ignored within the framework</u> of one-equation TKE schemes.

#### TKESV vs. One-Equation TKE Scheme (Draft Horse of Geophysical Turbulence Modelling)

Equation for  $<\theta'^2>$ 



Production = Dissipation (implicit in all models that carry the TKE equations only)

Equation for  $\langle w'\theta' \rangle$ 

$$\overline{w'\theta'} = -C_{\theta g} \tau_{\varepsilon} e \frac{\partial \overline{\theta}}{\partial z} + C_{\theta \varepsilon} \tau_{\varepsilon} g \sigma \overline{\theta'}^2$$

No way to get counter-gradient scalar fluxes in convective flows unless third-order scalar-variance transport is included (cf. turbulence schemes using "counter-gradient corrections" heuristically).

#### In Terms of Popular Mellor-Yamada Hierarchy of Second-Order Closures...

The hierarchy is based on the departure from isotropy considerations.

Level 2: all second moments are computed algebraically (productiondestruction equilibrium, assuming steady-state and homogeneity)

**Level 3**: TKE and scalar variances are computed prognostically (nonstationarity) with due regard for third-order transport terms (nonhomogeneity); all other second moments algebraically

Level 4: all second moments are computed prognostically

Level 2.5: TKE computed prognostically and all other second moments algebraically. Level 2.5 is an <u>inconsistent artificial construct</u> that cannot be derived from departure-from-isotropy considerations! (cf. original Mellor and Yamada, 1974, paper)

#### In Terms of Mellor-Yamada Hierarchy (cont'd)



#### Skewness-Dependent Parameterization of Third-Order Transport



Accounts for non-local transport due to coherent structures (convective plumes or rolls) – mass-flux ideas!

### **Mass-Flux Approach**

A top-hat representation of a fluctuating quantity (two- $\delta$ -function PDF)



#### **Mass-Flux Formulation in Terms of SOC**

Skewness of two- $\delta$ -function PDF (*a* is the updraught fractional area)

$$S_{\theta} \equiv \frac{\theta'^{3}}{\overline{\theta'^{2}}^{3/2}} = \frac{1 - 2a}{[a(1 - a)]^{1/2}}$$

 $S_{\theta}$  tends to  $\infty$  (- $\infty$ ) as *a* tends to 0 (1). Then

$$\overline{w'\theta'^2} = a(1-a)(1-2a)(w_u - w_d)(\theta_u - \theta_d)^2$$
$$= S_{\theta}\overline{\theta'}^2 \overline{w'\theta'}$$

# The mass-flux formulation recast in terms of the ensemble-mean quantities!

#### Sensitivity to Filter Scale (Resolution)

$$\overline{u_i'\theta'}^2 = -K\frac{\partial \theta'}{\partial x_i} + S_\theta \overline{\theta'}^{2} \overline{u_i'\theta'}, \quad S_\theta = \frac{\theta'}{\overline{\theta'}^{2}} \overline{\theta'}^{3/2}$$

As the resolution is refined, the SGS motions are (expected to be) increasingly Gaussian.

Then,  $S_{\theta} \rightarrow 0$  and the parameterization of the thirdorder transport term reduces to the down-gradient diffusion approximation.

#### Sensitivity to Filter Scale (Resolution)



#### **Closure for Skewness**

In order to determine skewness, we make use of the transport equation for the potential-temperature triple correlation

$$\frac{1}{3}\left(\frac{\partial}{\partial t} + \overline{u}_i \frac{\partial}{\partial x_i}\right)\overline{\theta'^3} = -\overline{u'_i}{\theta'^2}\frac{\partial\overline{\theta}}{\partial x_i} + \overline{\theta'^2}\frac{\partial}{\partial x_i}\overline{u'_i}{\theta'} - \frac{1}{3}\frac{\partial}{\partial x_i}\overline{u'_i}{\theta'^3} - \mathcal{E}_{\theta^3}$$

Using the mass-flux ideas, the fourth-order moment is closed through the temperature skewness (Gryanik and Hartmann 2002) – no need for equations of higher order!

$$\overline{u_i'\theta'^3} = 3\left(1 + \frac{1}{3}S_\theta^2\right)\overline{\theta'^2}\overline{u_i'\theta'}$$

### **Turbulence Anisotropy**



Much effort went into improving the treatment of TKE, but the Devil sits in the pressure terms in the (algebraic) equations for fluxes.

### **Coupling with Statistical Cloud Scheme**

Most statistical cloud schemes use at least two moments of distribution of  $\theta_l$  and  $q_t$ . For Gaussian cloud scheme, for example, the only predictor is the <u>normalized saturation deficit</u> that combines mean and variance.



$$Q_1 = \frac{q_t - q_s(T_l)}{\sigma_s},$$

$$\sigma_s^2 = a \left( \overline{q_t'^2} + P^2 \overline{\theta_l'^2} - 2P \overline{q_t' \theta_l'} \right)$$

A more accurate estimate of  $\sigma_s$  provided by a mixing scheme will (hopefully) lead to a better cloud forecast.

## Single Column Tests (summary)

- TKESV scheme is favourably tested through single-column numerical experiments (outperforms one-equation TKE scheme)
- Dry PBL: enhanced mixing, up-gradient heat transfer
- Cloudy PBLs (shallow cumuli, stratocumuli): better prediction of scalar variances and TKE, slight improvements with respect to the vertical buoyancy flux and the mean temperature and humidity

### **Dry Convective PBL**



Mean Temperature

#### **TKE and TKESV Schemes** vs. LES Data

Potential temperature minus its minimum value within the PBL. Black dotted curve shows LES data (Mironov et al. 2000), red – TKE scheme, blue – TKESV scheme.

### Dry Convective PBL (cont'd)



TKE (left panel) and  $\langle \theta'^2 \rangle$  (right panel) made dimensionless with  $w_*^2$  and  $\theta_*^2$ , respectively **Black dotted** curves show LES data, red – one-equation scheme, blue – two-equation scheme.

### **Shallow Cumulus Topped PBL**



Potential temperature variance (two left panels) and total water variance (two right panels) in BOMEX. Red – TKE scheme, blue – TKESV scheme. Black solid curves in the middle figures show LES data.

### **TKESV Scheme within COSMO**

- <u>Prognostic equations</u> for  $\langle u_i \rangle^2 >$  and for  $\langle \theta_l \rangle^2 >$ ,  $\langle q_t \rangle^2 >$  and  $\langle \theta_l \rangle q_t \rangle >$  <u>including third-order transport</u>
- <u>Algebraic (diagnostic) formulations</u> for scalar fluxes and Reynolds-stress components with due regard for anisotropy and for turbulence length scale (stability dependent)
- <u>Statistical SGS cloud scheme</u>, either Gaussian or skewed (ad hoc correction)
- Optionally, prognostic equation for <u>scalar skewness</u>



**Experiment** vs. **Operational** 

## Conclusions



- → A TKE-Scalar Variance (TKESV) mixing scheme is developed and favourably tested through single-column numerical experiments
- → The TKESV scheme is implemented into the limitedarea NWP model COSMO, results from parallel experiments look promising (improvements as to the 2m temperature and humidity and, to a lesser extent, to the fractional cloud cover)
- Implementation into the global NWP model ICON is planned
- Documentation of the TKESV scheme is in preparation



## **Future Challenges**



- Development of a three-moment (mean, variance, and skewness) statistical SGS cloud scheme that accounts for non-Gaussian effects, (A. Seifert and A. K. Naumann, HErZ on Cloud and Convection, Hamburg). Work is basically done.
- Coupling the skewness equations with the threemoment statistical cloud scheme.

Skewness-dependent "diffusion+advection" parameterizations of the thirdorder moments in the scalar-variance equations are developed and tested (optional within the TKESV scheme). These are, however, not recommended for the immediate use within COSMO due to numerical stability problems.



## **Future Challenges**



Improved coupling of the scalar-variance equations to the tiled surface scheme to better account for the effect of surface heterogeneity on the PBL structure and mixing (Mironov and Sullivan 2010, further co-operative work with Peter Sullivan, NCAR), use of PBL scalar variances in stochastic parameterizations.

Efforts go into the analysis of various flow regimes over heterogeneous surfaces (e.g. temperature-heterogeneous flat surface versus temperature-homogeneous surface with orographic features), and into the formulation of the surface boundary conditions for the scalar variances with due regard for the surface heterogeneity.







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#### **Supplementary Material**



#### Key Point: Modelling Pressure Redistribution (Scrambling) Terms in the Flux Budgets

Truncated (algebraic) equation for the scalar flux

$$0 = -\underbrace{\left(S_{ij} + W_{ij}\right)}_{kij} \overline{\theta'}_{ij} - \overline{u'_{i}u'_{k}} \frac{\partial \overline{\theta}}{\partial x_{k}} - \underbrace{g_{i}\alpha \overline{\theta'}^{2}}_{i} - \overline{\theta'} \frac{\partial p'}{\partial x_{i}}$$
known should be modeled  
From the Poisson equation 
$$\Pi_{\theta i} \equiv -\overline{\theta'} \frac{\partial p'}{\partial x_{i}} = \Pi_{\theta i}^{t} + \Pi_{\theta i}^{s} + \Pi_{\theta i}^{b} + \Pi_{\theta i}^{c} =$$

$$= -C_{t}^{\theta} \frac{\overline{u'_{t}\theta'}}{\tau_{\theta}} + \underbrace{\left(C_{s1}^{\theta}S_{ij} + C_{s2}^{\theta}W_{ij}\right)}_{ij} \overline{u'_{j}\theta'} + \underbrace{C_{b}^{\theta}g_{i}\alpha \overline{\theta'}^{2}}_{i}$$

Like terms can be collected  $\rightarrow$  linear model. However...

#### **Realizability Constraints in Anisotropic Limits**

$$\overline{u_i'\theta'} = \frac{\tau_\theta}{C_t^\theta} \left[ \left( \left(1 - C_{s1}^\theta\right) S_{ij} + \left(1 - C_{s2}^\theta\right) W_{ij} \right) \overline{u_j'\theta'} + \left(1 - C_b^\theta\right) \beta_i \overline{\theta'}^2 \right]$$

Near the wall or inversion:  $u'_i \to 0 \implies \overline{u'_i \theta'} \to 0$ 

 $C_{b}^{\theta} = const$  leads to a spurious generation of scalar (e.g. heat) flux!

Actually,  $C_{b}^{\theta}$  is a (complex) function of the governing parameters of the problem (departure-from-isotropy tensor, scalar flux vector, etc.).

 $C_b^{\theta} = const$  is not acceptable in case of stable stratification.  $C_b^{\theta}$  must approach 1 as  $w' \rightarrow 0$  (turbulence approaches a two-component limit).

In the TKESV scheme (Level 3)  $C_b^{\theta}$  can be made a linear function of anisotropy tensor without making the system of algebraic equations for fluxes non-linear.

### **Coupling with Statistical Cloud Scheme**



### **Coupling with Statistical Cloud Scheme**

For shallow cumulus regime (highly localized motions), the Gaussian distribution does not works well. Skewness is very important!

A three-moment (mean, variance, and skewness) statistical SGS cloud scheme that is based on the double Gaussian distribution and accounts for non-Gaussian effects (c/o Axel Seifert and Ann Kristin Naumann, Hans Ertel Centre on Cloud and Convection (HErZ), Hamburg) is developed.



Scalar variances and scalar skewness computed by the TKESV scheme are used as an input to the cloud scheme.

(Golaz et al., 2002)

#### **Remaining Problems and Future Challenges**

#### **Skewness-dependent "diffusion + advection" parameterizations** of the third-order moments in the scalar-variance equations

• The skewness-dependent parameterizations are developed, tested through single-column experiments, and are available as an option within the TKESV scheme. These parameterizations reduce numerical stability of the entire scheme (smaller time step is required) and are not recommended for immediate implementation into COSMO (cf. three-moment SGS cloud scheme).

#### **Coupling with the three-moment statistical cloud scheme**

• 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.

#### **Remaining Problems and Future Challenges**

# **Regularization of the pathological behaviour of stability functions in non-stationary conditions (growing turbulence)**

The problem is well-known and is recognized to be associated with the <u>truncation</u> of equations (<u>neglecting</u> of the terms that are responsible for <u>inhomogeneity</u> and <u>non-stationarity</u>).

The ways to handle it: either to regularize the solution (widely used, but too crude) or to regularize the equations (more mild and model-friendly).

The idea (Helfand & Labraga, 1988) is to re-insert into the algebraic equations the "transport" terms that would emulate what was neglected by the truncation.

In the Level 3 model, there is a possibility to do it in a more intelligent way because of an additional degree of freedom (scalar variance).

#### **Remaining Problems and Future Challenges**

Last but not least...

# **Regularization of the pathological behaviour of stability functions:** what is "pathological"?

The answer can be formulated in terms of <u>realizability</u> of a model:

a model is realizable if there exists a probability distribution with a given sequence of statistical moments predicted by the model (du Vachat, 1977). (In mathematics, it is referred as to moments problem.)

Example: criterium for the existence of PDF in the case of one fluctuating variable: given the sequence of the moments  $m_k$ ,

the matrix *H*, where  $H_{ij} = m_{i+j}$ , i+j=k, must be positive semi-definite.

(Non-negativity of variance follows from this more general condition.)

The requirement of realizability impose constraints on the moments.  $\rightarrow$  "pathology" may be strictly defined





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