Report from stay in Prague eTKE scheme and preparationd for TOMs

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eTKE scheme 1

eTKE scheme is an extension of pTKE scheme [10]. It replaces Louis stability functions F_m and F_h (for momentum and potential temperature, respectively) [13], [12] with new stability function, which are derived from TKE (Turbulence Kinetic Energy - E) equation (4). The idea is to have eTKE scheme equivalent to full TKE scheme for the non-discretised equations.

eTKE differs from full TKE scheme only in the two step computation of TKE equation (like in pTKE). This is done for three reasons: shallow convection parametrisation with Richardson number [7], antifibrilation scheme [1] and numerical stability, which we empirically see to be effectively better in the eTKE scheme than in the full TKE scheme. Both schemes are equivalent if shallow convection and antifibrilation scheme are switched off.

Stability functions F_m , F_h 1.1

For the terms I (wind shear), II (buoyancy), III(dissipation) in TKE equation we use extended expressions based on Cuxart, Bougeault and Redelsperger(CBR) turbulence scheme [4]:

$$I = -\overline{u'w'}\frac{\partial\overline{u}}{\partial z} - \overline{v'w'}\frac{\partial\overline{v}}{z} = \frac{4}{15}\frac{L_K}{C_m}\chi_3(Ri)\sqrt{E}\left[\left(\frac{\partial\overline{u}}{\partial z}\right)^2 + \left(\frac{\partial\overline{v}}{\partial z}\right)^2\right] \quad , \tag{1}$$

$$II = \frac{g}{\theta}\overline{\theta'w'} = -\frac{g}{\theta}\frac{2L_K}{3C_s}\sqrt{E}\frac{\partial\overline{\theta}}{\partial z}\phi_3(Ri) \quad , \tag{2}$$

$$III = -\epsilon = -C_{\epsilon} \frac{(E)^{\frac{3}{2}}}{L_{\epsilon}} \quad , \tag{3}$$

where Ri is gradient Richardson number, $\chi_3(Ri)$, $\phi_3(Ri)$ are stability functions, L_K and L_{ϵ} are mixing lengths and C_m , C_s and C_ϵ are closure constants. In original CBR scheme is $\chi_3(Ri)$ equal to 1.

The full TKE equation is:

$$\frac{dE}{dt} = -\frac{\partial}{\partial z} \left(\overline{E'w'} + \frac{\overline{p'w'}}{\rho} \right) + I + II + III \tag{4}$$

and in pTKE we have:

$$\frac{dE}{dt} = -\frac{\partial}{\partial z} \left(-K_E \frac{\partial E}{\partial z} \right) + \frac{1}{\tau_{\epsilon}} \left(\tilde{E} - E \right) \quad , \tag{5}$$

where $\tau_{\epsilon} = \frac{E}{\epsilon}$ and $\overline{E'w'} + \frac{\overline{p'w'}}{\rho} = -K_E \frac{\partial E}{\partial z}$. To have these two equations equivalent we need:

$$\tilde{E} = \frac{E}{\epsilon} (I + II) \tag{6}$$

If we use this condition, modified ¹ relations between TKE-mixing lengths L_K and L_{ϵ} and Prandtl-type mixing length l_m [14], [10]:

$$L_K C_K = \nu l_m \frac{f(Ri)^{\frac{1}{4}}}{\chi_3^{\frac{1}{2}}} \quad , \tag{7}$$

$$\frac{L_{\epsilon}}{C_{\epsilon}} = \frac{l_m}{\nu^3} \frac{\chi_3^{\frac{3}{2}}}{f(Ri)^{\frac{3}{4}}}$$
(8)

$$f(Ri) = \chi_3(Ri) - RiC_3\phi_3(Ri) \tag{9}$$

and the same scaling like in pTKE we get following form for stability functions F_m, F_h :

$$F_m(Ri) = \chi_3(Ri)\sqrt{f(Ri)} = \chi_3(Ri)\sqrt{\chi_3(Ri)(1-Ri_f)} \quad , \tag{10}$$

$$F_h(Ri) = \frac{\phi_3(Ri)}{\chi_3(Ri)} F_m(Ri) \quad , \tag{11}$$

where $\nu = (C_{\epsilon}C_K)^{\frac{1}{4}}$, C_K is closure constant, C_3 is the inverse of Prandtl number at neutrality and $Ri_f = Ri\frac{K_h}{K_m}$ is flux Richardson number (K_m and K_h are vertical exchange coefficients). These stability functions are used instead of Louis stability functions in computation of exchange coefficients K_m , K_h and also in computation of drag coefficients C_M , C_H [13], [12] (used at surface).

Modified relations between mixing lengths (7),(8) influences also relation for dissipation time scale τ_{ϵ} and auto-diffusion vertical coefficient for the TKE K_E^2 :

$$\tau_{\epsilon} = \frac{l_m}{\nu^3 \sqrt{E}} \frac{\chi_3(Ri)^{\frac{3}{2}}}{f(Ri)^{\frac{3}{4}}} \quad , \tag{12}$$

$$K_E = \frac{l_m \sqrt{E}}{\nu} \frac{f(Ri)^{\frac{3}{4}}}{\chi_3 (Ri)^{\frac{3}{2}}} \quad . \tag{13}$$

1.2 Vertical profile of Prandtl number at neutrality

Turbulent Prandtl number $(Prt = \frac{l_m}{l_h} \frac{F_m(Ri)}{F_h(Ri)} = \frac{1}{C_3} \frac{\chi_3(Ri)}{\phi_3(Ri)}, l_m$ and l_h are Prandtl mixing lengths for momentum and potential temperature, respectively) is an important characteristic of turbulent flow. In eTKE is the Prandtl number at neutrality Prt_0 determined by the ratio of mixing lengths $\frac{l_m}{l_h}$, but is also connected to the constant C_3 ³.

We have changed the vertical profile of Prt_0 to avoid inconsistencies of these two inputs: Prt_0 goes from unity at the surface (like in [2]) to $\frac{1}{C_3}$ in the free atmosphere.

This is done by computing first the vertical profile of the ratio $\frac{l_m}{l_h}$ with changed tuning constants $\lambda_m, \lambda_h, \beta_m, \beta_h$ in [2]:

$$l_{m/h} = \frac{\kappa z}{1 + \frac{\kappa z}{\lambda_{m/h}}} \left[\frac{1 + \exp\left(-a_{m/h}\sqrt{\frac{z}{H_{pbl}}} + b_{m/h}\right)}{\beta_{m/h} + \exp\left(-a_{m/h}\sqrt{\frac{z}{H_{pbl}}} + b_{m/h}\right)} \right]$$
(14)

(κ is Von Kármán constant, z is height, $a_{m/h}$, $b_{m/h}$ and $\lambda_{m/h}$ are tuning constants and H_{pbl} is PBL height)

¹There are 2 modification in comparison with relation used in pTKE. First is due $\chi_3(Ri) \neq 1$ and second one is caused by replacement of condition $f(Ri)\phi_m = 1$ by $\phi_m = \frac{1}{\chi_3(Ri)^{\frac{1}{2}}f(Ri)^{\frac{1}{4}}}$, which is derived from [3].

²Only τ_{ϵ} is modified directly by relation of mixing lengths. K_E is modified in order to keep ratio $\frac{1}{K_E}$ the same as in pTKE. This ensures that matrix of the solver is positive diagonally dominant [19].

³Value of constant C_3 is determined under the assumption, that turbulence is isotropic, which is valid in free atmosphere.

so, that we get:

$$\frac{\lambda_m}{\lambda_h} = \frac{1}{C_3} \quad , \tag{15}$$

$$\frac{\beta_m}{\beta_h} = 1 \quad . \tag{16}$$

And then the ratio $\frac{l_m}{l_h}$ is used to compute mixing length l_h from mixing length l_m . Calculation of l_m is not restricted to relation (14). We are especially interested in using mixing lengths, which are computed from TKE (L) and then converted with (7), (8):

$$L \equiv \sqrt{L_K L_\epsilon} = \frac{\nu}{C_K} l_m \frac{\chi_3(Ri)^{\frac{1}{2}}}{f(Ri)^{\frac{1}{4}}}$$
(17)

to Prandtl-type mixing length l_m . Note, that through (17) l_m becomes a function of Ri.

1.3 Stability functions χ_3 , ϕ_3

We used two sets of stability functions χ_3 , ϕ_3 :

1. modified⁴ CCH scheme [3], [9]:

$$\chi_3(Ri) = \frac{1 - \frac{Ri_f}{R}}{1 - Ri_f} =$$
(18)

$$= \frac{f(Ri)}{f(Ri).R+1-R} ,$$
 (19)

$$\phi_3(Ri) = \frac{1 - \frac{Ri_f}{Ri_{fc}}}{1 - Ri_f} =$$
(20)

$$= \left(1 - \frac{1 - Q}{f(Ri).R + 1 - R}\right) \frac{f(Ri)}{f(Ri).Q + 3\lambda_0 Ri} \quad , \tag{21}$$

$$Ri_f = \frac{C_3 Ri\phi_3(Ri)}{\chi_3(Ri)}, Ri_{fc} = \lim_{Ri \to \infty} Ri_f$$
(22)

$$(R = 1 - \frac{4}{\lambda_1} \left(\lambda_3^2 - \frac{\lambda_2^2}{3}\right), Q = 1 - 3\left(\lambda_3 - \frac{\lambda_2}{3}\right) \text{ and } \lambda_0 \text{ are constants [3]}),$$

2. fitted QNSE scheme [18], [9]:

for
$$Ri \ge 0$$
 $\chi_3(Ri) = \frac{1+0.75Ri(1+a.Ri)}{1+3.23Ri(1+a.Ri)}$, (23)

for
$$Ri < 0$$
 $\chi_3(Ri) = \frac{1 - b.Ri}{1 - (b - 2.48).Ri}$, (24)

where a = 13.0 and b = 4.16 are tuning constants.

Stability function $\phi_3(Ri)$ is computed from quadratic equation:

$$C_3 Ri\phi_3 (Ri)^2 - \left[\chi_3 (Ri) + \frac{C_3 Ri}{Ri_{fc}}\right]\phi_3 (Ri) + \chi_3 (Ri) = 0 \quad , \tag{25}$$

which was derived in modified CCH scheme, but we assume, that it is relevant also for QNSE scheme $^5.$

 $[\]overline{{}^4$ modification to avoid existence of critical gradient Richardson number Ri_{cr}

⁵Our assumption is confirmed by the fact, that resulting ϕ_3 function from (25) with fitted $\chi_3(Ri)$ function (18) for QNSE is very close to 'original' QNSE function ϕ_3 [17].

1.4 'Dry' antifibrilation scheme

The 'dry' (antifibrilation scheme without taking into account the shallow convection parametrisation - [1]) antifibrilation (**AF**) scheme depends on the shape of stability functions F_m and F_h . So we changed the computation of coefficients α_u a α_θ (which are used for computation of AF coefficients *PXUROV*, *PXTROV*, *PXPTKEROV*) by using new stability functions F_m and F_h in relations:

$$\alpha_u = \frac{Ri}{F_m(Ri)} \left(\frac{dF_m(Ri)}{dRi}\right) \quad , \tag{26}$$

$$\alpha_{\theta} = \frac{Ri}{F_h(Ri)} \left(\frac{dF_h(Ri)}{dRi} \right) \quad . \tag{27}$$

New stability functions F_m and F_h don't meet the required conditions for use of AF scheme [1] for all Ri:

$$K_m \ge \frac{K_h}{3}$$
 or $\alpha_\theta > -1$ (for $Ri > 0$) , (28)

$$-2 < (\alpha_u, \alpha_\theta) < 1 , \qquad (29)$$

$$2 \quad < \quad 3 - 2.\alpha_u + \alpha_\theta \quad , \tag{30}$$

$$0 < 2 - 3.\alpha_u + 2.\alpha_\theta \le 2$$
 , (31)

so we restricted the use of AF scheme only to intervals when they are met.

This change in AF scheme is made in free atmosphere (ACCOEFK) and also at surface(ACHMT).

2 Preparation for TOMs

We would like to introduce TOMs (Third Order Moments) in to the turbulent scheme [9]. To proceed to this step we need to change the eTKE scheme so, that there are no modification of exchange coefficients K_m and K_h after their calculation from stability functions F_m and F_h :

$$K_m = l_m^2 \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 \right]^{\frac{1}{2}} F_m(Ri) \quad , \tag{32}$$

$$K_h = l_m l_h \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 \right]^{\frac{1}{2}} F_h(Ri) \quad .$$
(33)

Currently are in the scheme two such modifications of exchange coefficients: 'moist' AF scheme and parametrisation of moist gustiness.

2.1 'Moist' antifibrilation scheme

Parametrisation of shallow convection with modified Ri^* [7] can cause nonlinear instabilities in diffusion equation ('fibrillations'). These instabilities are treated in 'moist' AF scheme by modification of exchange coefficients from $K_{m/h}$ to $K'_{m/h}$:

$$K'_{m/h}(Ri_d, Ri^*) = K_{m/h}(Ri_d) + \frac{K_{m/h}(Ri^*) - K_{m/h}(Ri_d)}{1 + (\beta - 1)(K_{m/h}(Ri^*) - K_{m/h}(Ri_d))\Delta t} \quad , \tag{34}$$

where β is decentering factor, Ri_d is 'dry' (without shallow convection parametrisation) Richardson number and Δt is time-step.

We have shifted the 'moist' AF scheme in to the computation of Richardson number Ri', which means, that we use Ri' for computation of stability functions χ_3 and ϕ_3 and we no longer need to use 'moist' AF scheme on exchange coefficients.

Derivation of Ri' begins with replacement of expression (34) for exchange coefficients with expression for stability functions:

$$F_{m/h}(Ri') = F'_{m/h}(Ri_d, Ri^*) = F_{m/h}(Ri_d) + \frac{F_{m/h}(Ri^*) - F_{m/h}(Ri_d)}{1 + (\beta - 1)(F_{m/h}(Ri^*) - F_{m/h}(Ri_d))l_m l_h \sqrt{\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2} \Delta t} \quad .$$
(35)

Then we inverted stability function F_h (11)⁶ and expressed the modified Ri'.

2.1.1 Modified CCH scheme

For modified CCH scheme we used a special form of stability functions derived by Daan Degrauwe [5]:

$$\phi_3 = \frac{S-1}{Ri_{fc}.S-1} \quad , \tag{36}$$

$$\chi_3 = \frac{\frac{S}{\sigma} - 1}{Ri_{fc} \cdot S - 1} \quad , \tag{37}$$

$$S = \frac{Ri_f}{Ri_{fc}} = \frac{1}{2} \left[\sigma(1+\rho) - \sqrt{(1+\rho)^2 \sigma^2 - 4\rho\sigma} \right] , \qquad (38)$$

$$\sigma = \frac{R}{Ri_{fc}} \quad , \quad \rho = \frac{C_3 Ri}{Ri_{fc}} \quad . \tag{39}$$

In this form is stability function F_h expressed following:

$$F_h = \phi_3 \sqrt{\chi_3(1 - Ri_f)} = \frac{S - 1}{Ri_{fc} \cdot S - 1} \sqrt{\frac{S}{\sigma}} - 1 \quad . \tag{40}$$

Inversion of (40) with respect to S leads to cubic equation for S with only one real root for all F_h :

$$0 = S^{3} + \left(\left(F_{h}^{2} R_{i_{fc}}^{2} - 1 \right) \sigma - 2 \right) S^{2} + \left(\left(2 - 2 F_{h}^{2} R_{i_{fc}} \right) \sigma + 1 \right) S + \left(F_{h}^{2} - 1 \right) \sigma \quad .$$
(41)

When we solve S, we can compute Ri' from (38):

$$Ri' = \frac{Ri_{fc}}{C_3} \frac{S - \sigma}{\sigma} \frac{S - \sigma}{S - 1} \quad . \tag{42}$$

2.1.2 QNSE scheme

QNSE scheme has more complicated form of stability function $F_h(\chi_3, \phi_3)$. We are not able to invert it analytically. So we fitted QNSE functions χ_3 and ϕ_3 with modified CCH functions $(R, C_3$ - functions of Ri, $Ri_{fc} = 0.377$, $\nu = 0.464$) and used them to invert F_h function (like in 2.1.1). Note, that this fit of χ_3 and ϕ_3 functions is used only for computation of Ri'.

2.2 Moist gustiness modification

Moist gustiness parametrisation [8] multiplies exchange coefficients $K_{m/h}$ and drag coefficients $C_{M/H}$ by the factor:

$$\gamma^{PRC} = \sqrt{1 + \left(\left(\frac{J_{Pr}}{J_{Pr} + J_{Pr}^0}\right)^{\gamma} \tilde{U}\right)^2 \frac{K_m \cdot \sqrt{\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2}}{\rho} \quad , \tag{43}$$

where J_{Pr} is precipitation flux, J_{Pr}^0 is typical steadily strong precipitation flux, \tilde{U} is typical surface friction velocity, $\gamma = 0.8$ is a tuning constant and ρ is density.

We have shifted this modification from exchange coefficients to mixing lengths, so that mixing lengths l_m and l_h are multiplied by $\sqrt{\gamma^{PRC}}$ before they enter computation of exchange coefficients K_m and K_h (32), (33).

Direct effect of moist gustiness on exchange coefficients is the same as by multiplying them directly, but mixing lengths influence also the TKE solver [19] (through τ_{ϵ} , \tilde{E} and K_E) and so the values of 'prognostic' exchange coefficients K_m and K_h .

Modification of moist gustiness modification through mixing lengths l_m and l_h affects only computation of exchange coefficients K_m , K_h . We didn't change computation at the surface (drag coefficients $C_{M/H}$).

⁶There are two ways how to derive Ri': through F'_m or F'_h . These two approaches give different results, but we logically demand, that Ri' has a unique definition. We decided to use the definition through F'_h .

2.3 Mixing lengths

Modification in 'moist' AF scheme (with Ri' in (7)) and in moist gustiness parametrisation influence the values of mixing lengths l_m and l_h . But mixing lengths appear in both schemes as inputs (35), (43) (in K_m). To avoid iterative methods we simply use mixing length l_m^d without moist gustiness correction and without shallow convection parametrisation (influence through Ri) in both schemes. This means we have to compute mixing lengths twice per time-step: before computation of $Ri' - l_m^d$ and before making moist gustiness correction - l_m'' (with shallow convection parametrisation) (see Figure 1).

3 Shallow convection cloudiness

Richardson number Ri' is a result of shallow convection parametrisation and 'moist' AF scheme. Ri' should be limited by Ri_d (no clouds in grid box) and Ri_m (Richardson number for saturated air - 100 % cloudiness in grid box) [6]:

$$Ri_{m} = g \frac{1 + \frac{L_{v} \cdot q_{w}}{R.T}}{1 + \left(\frac{\epsilon \cdot L_{v}^{2} \cdot q_{w}}{c_{p} \cdot R.T^{2}}\right)} \left(\frac{d\ln\theta}{dz} + \frac{L_{v}}{c_{p} \cdot T} \frac{dq_{w}}{dz}\right) \frac{1}{\left(\frac{\partial\overline{u}}{\partial z}\right)^{2} + \left(\frac{\partial\overline{v}}{\partial z}\right)^{2}} \quad , \tag{44}$$

where q_w is specific moisture corresponding to wet bulb temperature, L_v is latent heat of vaporization, R is gas constant, c_p is specific heat capacity and ϵ is ratio of gas constants for dry air and water vapor.

We defined shallow convection cloudiness N_{cvpp} by the 'position' of Ri' in interval $\langle Ri_d, Ri_m \rangle$. To ensure, that N_{cvpp} is in the range $\langle 0, 1 \rangle$ we limit Ri' by Ri_m and Ri_d and get Ri'':

$$Ri'' = \min(\max(Ri_d, Ri'), Ri_m) \quad . \tag{45}$$

Shallow convection cloudiness N_{cvpp} is then defined as:

$$N_{cvpp} = \frac{Ri'' - Ri_d}{Ri_m - Ri_d} \quad . \tag{46}$$

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$L, Ri_d \rightarrow l_m^d$	Mixing length
$l_m^d, Prt_0 \to l_h^d$	Vertical profile of Prt_0
$\begin{matrix} \mathbf{k} \\ Ri_d, Ri^*, l_m^d, l_h^d \to Ri' \end{matrix}$	'Moist' AF scheme
$\begin{matrix} \downarrow \\ Ri', Ri_m \to Ri'', N_{cvpp} \end{matrix}$	Shallow convection cloudiness
$Ri'', l_m^d, J_{Pr} \to \gamma^{PRC}$	Moist gustiness correction - computation
$L, Ri'' \rightarrow l''_m$	Mixing length
$l''_m, \gamma^{PRC} \to l''^{PRC}_m$	Moist gustiness correction - application
$l_m^{\prime\prime PRC}, Prt_0 \to l_h^{\prime\prime PRC}$	Vertical profile of Prt_0
$ \begin{array}{ccc} & & \\ Ri_d \to \chi_3(Ri_d), \phi_3(Ri_d) \to \\ F_m(Ri_d), F_h(Ri_d) \end{array} $	Stability functions
$F_m(Ri_d), F_h(Ri_d) \to \widetilde{C_M}, \widetilde{C_H}$	Drag coefficients C_M, C_H
$Ri_d \to \alpha_u, \alpha_\theta$	'Dry' AF scheme - 1
$ \overbrace{\widetilde{C_M}, \widetilde{C_H}, \alpha_u, \alpha_\theta}^{\Psi} \rightarrow PXDROV, PXHROV $	'Dry' AF scheme - 2
$ \begin{array}{cccc} $	Stability functions
$ \begin{array}{c} \overbrace{F_m(Ri''), F_h(Ri''), l_m''^{PRC}, l_h''^{PRC}}_{K_m, \widetilde{K_h}} \rightarrow \end{array} $	'Static' exchange coefficients $\widetilde{K_m}$, $\widetilde{K_h}$
$Ri'' \to \alpha_u, \alpha_\theta$	'Dry' AF scheme - 1
$\widetilde{K_m}, \widetilde{K_h}, \alpha_u, \alpha_\theta \to PXUROV, PXTROV, PXPTKEROV$	'Dry' AF scheme - 2
$\chi_{3}(Ri''), \phi_{3}(Ri''), l_{m}''^{PRC} \to \tau_{\epsilon}, \tilde{E}, K_{E}$	Preparation for TKE solver
$\checkmark \qquad \qquad$	TKE solver

Figure 1: Draft of turbulent scheme