"New" ACCOEFK subroutine in pTKE parametrisation scheme

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Pseudo-prognostic TKE scheme (hereafter pTKE) is an extension of the Louis type vertical diffusion scheme. pTKE scheme consists of two parts:

- 1. the static part the 'static' computation of turbulent exchange coefficients (subroutine ACCOEFK)
- 2. the prognostic part modifies the 'static' exchange coefficients with prognostic TKE equation (in ACDIFUS subroutine).

This document describes an alternative to currently used static part in pTKE scheme. 'New' approach is based on TKE (Turbulent Kinetic Energy) equation for TKE at stationary equilibrium.

1 Prognostic part

For better understanding of pTKE scheme [3] [9], we shortly summarize:

1.1 Input/output of prognostic part

Inputs for the prognostic part are:

• $\tilde{K}_m, \tilde{K}_h, \tilde{K}_n$ - 'static' exchange coefficients for momentum, potential temperature(also specific moisture) and for momentum at neutrality,

- l_m Prandtl-type mixing length for momentum and
- TKE(e) -Turbulent Kinetic Energy

Outputs are the modified exchange coefficients, which are used for computation of turbulent fluxes and the tendency of TKE.

1.2 Prognostic TKE equation

Besides the balance between wind shear and buoyancy production/destruction terms and the dissipation term enables the prognostic TKE equation also advection, horizontal diffusion and the vertical auto-diffusion of the TKE. To use TKE equation we need to link our inputs (similarity laws) with the input parameters for TKE equation (TKE formalism):

- TKE,
- K_E -vertical exchange coefficient for TKE and
- τ_{ϵ} dissipation time scale.

1.3 Link between similarity laws and TKE formalism

The method proposed by Redelsperger, Mahé and Carlotti(2001) [7] is used to provide this link. We have:

$$K_m = \nu l_m \Phi_L(\frac{K_m}{K_n}) \sqrt{e} \tag{1}$$

$$\frac{1}{\tau_{\epsilon}} = \nu^3 \frac{1}{l_m \Psi_L(\frac{K_m}{K_n})} \tag{2}$$

where $\nu^4 = C_K * C_{\epsilon}$ (C_K and C_{ϵ} are constants) and $\Psi_L(\frac{K_m}{K_n})$ and $\Phi_L(\frac{K_m}{K_n})$ are stability function in expressions for sub-grid-scale lengths:

$$L_K = Az\Phi_L(\phi_E, \phi_m) \tag{3}$$

$$L_{\epsilon} = Az\Psi_L(\phi_E, \phi_m) \tag{4}$$

where ϕ_E, ϕ_m are Monin-Obukhov stability functions.

To make the relations (1) and (2) free from stability functions new variables were introduced to the scheme - K_* and ν_* :

$$\nu_* = \frac{\nu}{(\Psi_L)^{\frac{1}{3}}}$$
(5)

$$K_* = \frac{K_m}{\Phi_L(\Psi_L)^{\frac{1}{3}}}$$
(6)

Two hypotheses has been made for Monin-Obukhov stability functions: $f\phi_m = 1$ and $\phi_m^2 = \frac{K_n}{K_m}$. We get:

$$\nu_* = \frac{\nu}{\phi_E \phi_m^2} \approx \nu \approx 0.52 \tag{7}$$

$$K_* = \sqrt{K_n K_m} \tag{8}$$

1.4 Link to output

 \tilde{K}_* is computed from the 'static' exchange coefficients \tilde{K}_m and \tilde{K}_n . This is used to estimate parameters for the TKE equation. K_* is calculated from the 'new' TKE, which is given by TKE equation. At this point we need to make the last step from the K_* and \tilde{K}_* exchange coefficients to the 'new' exchange coefficients K_m and K_h (output of pTKE):

$$K_m = K_* \frac{\tilde{K}_m}{\tilde{K}_*} \tag{9}$$

$$K_h = K_* \frac{\tilde{K}_h}{\tilde{K}_*} \tag{10}$$

2 Static part - 'new' ACCOEFK

First we describe the 'old' ACCOEFK:

2.1 'Old' ACCOEFK subroutine

Subroutine ACCOEFK [5] computes 'static' exchange coefficients and is based on 'Louis' technique [8]:

$$\tilde{K}_m = l_m l_m \left[\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 \right]^{\frac{1}{2}} F_m(Ri)$$
(11)

$$\tilde{K}_{h} = l_{m} l_{h} \left[\left(\frac{\partial \overline{u}}{\partial z} \right)^{2} + \left(\frac{\partial \overline{v}}{\partial z} \right)^{2} \right]^{\frac{1}{2}} F_{h}(Ri)$$
(12)

$$\tilde{K}_N = l_m l_m \left[\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 \right]^{\frac{1}{2}}$$
(13)

where $F_m(Ri)$ and $F_h(Ri)$ are shaping stability functions:

-stable case:

$$F_m(Ri) = \frac{1}{1 + \frac{2bRi}{\sqrt{1 + \frac{d}{k}Ri}}}$$
(14)

$$F_h(Ri) = \frac{1}{1 + 3bRi\sqrt{1 + dkRi}}$$
(15)

-unstable case:

$$F_m(Ri) = 1 - \frac{2bRi}{1 + 3bc\sqrt{\frac{|Ri|}{27}} \left(\frac{l_m}{z+z_0}\right)^2}$$
(16)

$$F_h(Ri) = 1 - \frac{3bRi}{1 + 3bc\sqrt{\frac{|Ri|}{27}} \left(\frac{l_h}{z + z_{0h}}\right) \left(\frac{l_m}{z + z_0}\right)}$$
(17)

where b,c,d,k are constants and z_0 and z_{0h} are roughness lengths for momentum and potential temperature, respectively.

2.2 'New' ACCOEFK subroutine

'New' ACCOEFK will use TKE equation for TKE at stationary equilibrium $(\frac{\partial e}{\partial t} = 0)$ and by using only three terms on the rhs of the TKE equation: wind shear(I), buoyancy(II) production/destruction term and the dissipation term(III) for estimation of 'static' exchange coefficients:

$$0 = I(\tilde{e}) + II(\tilde{e}) + III(\tilde{e})$$
(18)

where \tilde{e} is TKE at stationary equilibrium. The omitted terms on the rhs of full TKE equation will be added later in the prognostic part of pTKE.

We will use following expressions for I, II and III from the Cuxart, Bougealt and Redelsperger(CBR) turbulence scheme [2]:

$$I = -\overline{u'w'}\frac{\partial\overline{u}}{\partial z} - \overline{v'w'}\frac{\partial\overline{v}}{z} = \frac{4}{15}\frac{L}{C_m}\sqrt{e}\left[\left(\frac{\partial\overline{u}}{\partial z}\right)^2 + \left(\frac{\partial\overline{v}}{\partial z}\right)^2\right]$$
(19)

$$II = \frac{g}{\theta_r ef} \overline{\theta'w'} = -\frac{g}{\theta_{ref}} \frac{2L}{3C_s} \sqrt{e} \frac{\partial\theta}{\partial z} \phi_3(Ri)$$
(20)

$$III = -C_{\epsilon} \frac{(e)^{\frac{1}{2}}}{L}$$
(21)

where L is the mixing length. We suggest that $L/l_m = const. \phi_3(Ri)$ is stability function (see [7]):

$$\phi_3(Ri) = \frac{1}{1 + \frac{C_4 Ri}{f(Ri)}}$$
(22)

$$f(Ri) = \frac{1}{2} \left(1 - (C_3 + C_4)Ri + \sqrt{\left[(1 - (C_3 + C_4)Ri)^2 + 4C_4Ri \right]} \right)$$
(23)

$$C_3 = \frac{C_H}{C_K} \tag{24}$$

$$C_4 = \frac{C_H C_\epsilon}{C_K C_\theta} \tag{25}$$

where $C_H, C_K, C_m, C_s, C_\theta, C_\epsilon$ are closure constants and Ri is Richardson number, that will be estimated the same way as in the 'old' ACCOEFK.

We can solve (18) analytical. First we substitute $\sqrt{\tilde{e}} = X$ and write (18)) this way:

$$0 = A(L, \frac{\partial \overline{u}}{\partial z})X + B(L, \frac{\partial \overline{\theta}}{\partial z}, Ri)X + C(L)X^3$$
(26)

We get 3 solutions:

$$X_1 = 0 \quad X_2 = -\sqrt{\frac{D}{C}} \qquad X_3 = \sqrt{\frac{D}{C}}$$
(27)

where D=-(A+B). First solution is trivial. TKE is a real positive number, so the term $\frac{D}{C}$ must be positive or zero. We get :

$$\tilde{e} = \frac{D}{C} \ge 0 \tag{28}$$

$$= \frac{L^2}{C_{\epsilon}} \left(\frac{4}{15} \frac{1}{C_m} \left[\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 \right] - \frac{g}{\theta_{ref}} \frac{2}{3C_s} \frac{\partial \overline{\theta}}{\partial z} \phi_3(Ri) \right)$$
(29)

We use the definition of the (bulk) Richardson number Ri:

$$Ri = \frac{g}{\theta_{ref}} \frac{\frac{\partial \theta}{\partial z}}{\left[\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 \right]}$$
(30)

to eliminate $\frac{g}{\theta_{ref}} \frac{\partial \overline{\theta}}{\partial z}$ in (29). Additionally we use these relations for constants C_s and C_m :

$$C_K = \frac{4}{15C_m} \tag{31}$$

$$C_s = \frac{2}{3C_3C_K} \tag{32}$$

We get:

$$\tilde{e} = \frac{L^2 C_K}{C_{\epsilon}} \left(1 - Ri C_3 \phi_3(Ri)\right) \left[\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2 \right]$$
(33)

'Static' exchange coefficients will be then computed following:

$$\tilde{K}_m = \frac{4L}{15C_m}\sqrt{\tilde{e}} = C_K L \sqrt{\tilde{e}}$$
(34)

$$\tilde{K}_h = \frac{2L}{3C_s} \phi_3(Ri) \sqrt{\tilde{e}} = C_3 C_K \phi_3(Ri) L \sqrt{\tilde{e}}$$
(35)

In neutral case $(Ri = 0, \phi_3(Ri = 0) = 1)$ we get for $\tilde{K}_m(Ri = 0) = \tilde{K}_N$:

$$\tilde{K}_{N} = C_{K}L_{\sqrt{\frac{L^{2}C_{K}}{C_{\epsilon}}\left[\left(\frac{\partial\overline{u}}{\partial z}\right)^{2} + \left(\frac{\partial\overline{v}}{\partial z}\right)^{2}\right]}}$$
(36)

$$= \left(L\left(\frac{C_{\epsilon}}{C_{K}^{3}}\right)^{-\frac{1}{4}}\right)^{2} \left[\left(\frac{\partial\overline{u}}{\partial z}\right)^{2} + \left(\frac{\partial\overline{v}}{\partial z}\right)^{2}\right]^{\frac{1}{2}}$$
(37)

$$= l_m l_m \left[\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 \right]^{\frac{1}{2}}$$
(38)

Relation for $L(l_m)$ is:

$$L = l_m \left(\frac{C_{\epsilon}}{C_K^3}\right)^{\frac{1}{4}}$$
(39)

Now we can write 'new' stability functions F_m and F_h , which are functions of Richardson number only:

$$F_m(Ri) = \frac{\tilde{K}_m}{\tilde{K}_m(Ri=0)} = \frac{\tilde{K}_m}{\tilde{K}_N}$$
$$= \sqrt{(1 - RiC_3\phi_3(Ri))} = \sqrt{f(Ri)}$$
(40)

$$F_{h}(Ri) = \frac{K_{h}}{\tilde{K}_{h}(Ri=0)} = \frac{K_{h}}{C_{3}\tilde{K}_{N}} = C_{3}\phi_{3}(Ri)\frac{1}{C_{3}}\sqrt{(1-RiC_{3}\phi_{3}(Ri))}$$
$$= \phi_{3}(Ri)\sqrt{f(Ri)} = \phi_{3}(Ri)F_{m}(Ri)$$
(41)

 C_3 and C_4 are the only tuning constant in the computation of F_m and F_h .

2.3 Corrections for computation of stability functions

We will rewrite $\phi_3(Ri)$ for computation following:

$$\phi_3(Ri) = \frac{f}{f + C_4 Ri} \tag{42}$$

We will prove that the term $f + C_4 Ri$ is always positive for $Ri \leq 0$. We suggest that $C_3 > 0$ and $C_4 > 0$:

$$f + C_4 Ri = \frac{1}{2} (1 - (C_3 + C_4)Ri + \sqrt{(1 - (C_3 + C_4)Ri)^2 + 4C_4Ri} + 2C_4Ri)$$

+2C_4Ri)
$$= \frac{1}{2} \left(1 + (C_4 - C_3)Ri + \sqrt{(1 - (C_3 + C_4)Ri)^2 + 4C_4Ri} \right) (44)$$

We rewrite the term under square root:

$$(1 - (C_3 + C_4)Ri)^2 + 4C_4Ri = 1 - 2(C_3 + C_4)Ri + (C_3 + C_4)^2Ri^2(45) +4C_4Ri = 1 + 2(C_3 + C_4)Ri + (C_3 + C_4)^2Ri^2(46) -4C_3Ri > (1 + (C_3 + C_4)Ri)^2$$
(47)

For $Ri \leq -\frac{1}{C_3+C_4}$:

$$f + C_4 Ri > \frac{1}{2} (1 + (C_4 - C_3)Ri - (1 + (C_3 + C_4)Ri))$$
 (48)

>
$$\frac{1}{2}(-2C_3Ri) > 0$$
 (49)

For
$$0 \ge Ri > -\frac{1}{C_3 + C_4}$$
:
 $f + C_4 Ri > \frac{1}{2} (1 + (C_4 - C_3)Ri + (1 + (C_3 + C_4)Ri))$ (50)

>
$$\frac{1}{2}(2+2C_4Ri) > 0$$
 for $Ri > -\frac{1}{C_4}$ (51)

$$Ri > -\frac{1}{C_3 + C_4} > -\frac{1}{C_4}$$
(52)

For Ri > 0 exists a risk that the term $f + C_4Ri$ could be equal zero, when f(Ri) < 0. f(Ri) < 0 could be also a problem in the computation of the function $F_m = \sqrt{f(Ri)}$. We calculate limits for f(Ri):

$$f(Ri) = 0.5(X + \sqrt{X^2 + 4C_4Ri}) \qquad X = 1 - (C_3 + C_4)Ri$$
(53)

$$X \to \infty \text{ for } Ri \to -\infty \quad f(Ri) \to \infty \text{ for } Ri \to -\infty$$
 (54)

$$X \to -\infty \quad \frac{X}{Ri} \to -(C_3 + C_4) \quad for \quad Ri \to \infty$$
 (55)

$$f(Ri) = 0.5(X + \sqrt{X^2 + 4C_4Ri})\frac{\sqrt{X^2 + 4C_4Ri} - X}{\sqrt{X^2 + 4C_4Ri} - X}$$
(56)

$$f(Ri) = 0.5 \frac{4C_4Ri}{\sqrt{X^2 + 4C_4Ri} - X}$$
(57)

$$f(Ri) = \frac{2C_4}{\sqrt{\left(\frac{X}{Ri}\right)^2 + \frac{4C_4}{Ri} - \frac{X}{Ri}}}$$
(58)

$$f(Ri) \to \frac{2C_4}{2(C_3 + C_4)} = \frac{C_4}{(C_3 + C_4)} > 0 \text{ for } Ri \to \infty$$
 (59)

f(Ri) is always greater then 0.

2.4 Modifications in ACHMT subroutine

The computation of drag coefficients PCD (for wind components) and PCH (for temperature and humidity) [5] is related to the computation of vertical exchange coefficients through the stability functions F_m and F_h :

$$PCD = PCDN.F_m$$
 (60)

$$PCH = ZCDNH.F_h$$
 (61)

where PCDN and ZCDNH are drag coefficients at neutrality.

We replace the 'old' stability functions with the 'new' stability functions.

2.5 Asymptotic features of stability functions

Two necessary conditions for the asymptotic behavior of stability functions have to be met for stability functions [4] [6] :

I. an asymptotic value of the sensible heat flux:

$$\overline{\theta'w'} = l_m l_h \sqrt{\left[\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2\right]} \frac{\partial \overline{\theta}}{\partial z} F_h(Ri) \to const$$
(62)

when
$$\sqrt{\left[\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2\right]} = const$$
 and $\frac{\partial \overline{\theta}}{\partial z} \to \infty$ (63)

II. and convergent critical Richardson flux number Ri_f independent with respect to the critical Richardson number when $Ri \to \infty$:

$$Ri_{f} = \frac{g}{\theta_{ref}} \frac{\overline{\theta'w'}}{\overline{u'w'}\frac{\partial\overline{u}}{\partial z} + \overline{v'w'}\frac{\partial\overline{v}}{\partial z}} = R_{i}\frac{K_{h}}{K_{m}} \to const$$
(64)

when
$$Ri \to \infty$$
 (65)

2.5.1 'Old' stability functions - usage of the critical Richardson number

Asymptotic behavior of 'old' stability functions is modified by a limitation of Richardson number to parameter Ri_c - critical Richardson number [4] [6]:

$$R_i' = \frac{R_i}{\left(1 + \alpha \frac{R_i}{Ri_c}\right)^{\frac{1}{\alpha}}} \tag{66}$$

where vertical profile of Ri_c is given by:

$$Ri_c = \frac{Ri_c^{\infty}}{1 + (U_l - 1)(\frac{l_h}{\kappa(z + z_{0H})})^{USURICE}}$$
(67)

and coefficient α is:

$$\alpha = 1 \qquad \text{for momentum} \tag{68}$$

$$\alpha = \frac{3Ri + Ri_d}{Ri + Ri_d} \qquad \text{for temperature} \tag{69}$$

 Ri_d is tunable parameter with vertical profile:

$$Ri_{d} = \frac{Ri_{d}^{\infty}}{\left(1 + \frac{PBLH^{2}*\sqrt{3}}{(z+z_{0H})(z+z_{0})}\right)^{USURIDE}}$$
(70)

where PBLH is height of PBL. Ri_d^{∞} , Ri_c^{∞} , U_l , USURICE and USURIDE are parameters.

2.5.2 'New' stability functions

We will investigate the asymptotic behavior of 'new' stability functions.

I. We rewrite the sensible heat flux $\overline{\theta' w'}$:

$$\overline{\theta'w'} = K_1 RiF_h(Ri) = K_1 Ri\phi_3(Ri) \sqrt{(f(Ri))}$$
(71)

where

$$K_1 = \frac{\theta_{ref}}{g} l_m l_h \left[\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 \right]^{\frac{3}{2}}$$
(72)

and calculate limit for term $Ri\phi_3(Ri)$

$$Ri\phi_{3}(Ri) = \frac{Rif}{f + C_{4}Ri} = \frac{1}{\frac{1}{Ri} + \frac{C_{4}}{f}} \rightarrow \frac{1}{C_{3} + C_{4}}$$

$$for \quad \frac{\partial\overline{\theta}}{\partial z} \rightarrow \infty \quad .$$
(73)

Then

$$\overline{\theta'w'} \to \frac{K_1}{C_3 + C_4} = const \tag{74}$$

when

$$\sqrt{\left[\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2\right]} = const \qquad \text{and} \qquad \frac{\partial \overline{\theta}}{\partial z} \to \infty$$
(75)

II. We calculate the limit for the Richardson flux number Ri_f :

$$Ri_f = R_i \frac{K_h}{K_m} = R_i C_3 \phi_3 \to \frac{C_3}{C_3 + C_4} \quad for \quad R_i \to \infty$$
(76)

We can see that both necessary conditions for the asymptotic behavior of stability functions are met without limitation of Richardson number to critical Richardson number Ri_c .

2.6 Tuning parameters C_3 and C_4

2.6.1 Vertical profile of C₃

 $\frac{1}{C_3}$ is actually the turbulent Prandtl number at neutrality $Pr_T(Ri = 0)$. In 'old' ACCOEFK it is assumed that:

$$Pr_T(Ri=0) = 1$$
 at surface (77)

$$Pr_T(Ri=0) = \frac{l_m}{l_h}$$
 above the surface (78)

We need $Pr_T(Ri = 0)$ to depend on height in appropriate way, so we first modify vertical profiles of mixing lengths l_m , l_h in ACMIXLENZ so, that:

$$\frac{l_h}{l_m} = 1$$
 at surface (79)

$$\frac{l_h}{l_m} = C_{3free} = \frac{3\Pi}{4}$$
 above the PBL (80)

and then we compute C_3 in ACCOEFK on every level before the computation of F_m and F_h as:

$$C_3 = \frac{l_h}{l_m}.$$
(81)

This procedure gives us also a way how to bind l_m and l_h and get l_h as function of l_m .

Modification of profiles can be done via the choices of shaping constants $\lambda_m, \lambda_h, \beta_m, \beta_h$ in subroutine ACMIXLENZ, where:

$$l_{m/h} = \frac{\kappa z}{1 + \frac{\kappa z}{\lambda_{m/h}} \left[\frac{1 + e^{\left(-a_{m/h} \sqrt{\frac{z}{H_{pbl}}} + bm/h}\right)}{\left(\frac{1 + e^{\left(-a_{m/h} \sqrt{\frac{z}{H_{pbl}}} + bm/h}\right)}{\beta_{m/h} + e^{\left(-a_{m/h} \sqrt{\frac{z}{H_{pbl}}} + bm/h\right)}} \right]}$$
(82)

where $a_{m/h}, b_{m/h}$ are tuning constants and H_{pbl} is PBL height.

We force the vertical profile of l_m and l_h by two conditions:

$$\frac{l_h}{l_m} \to \frac{\lambda_h}{\lambda_m} \frac{\beta_h}{\beta_m} = C_{3free} \quad \text{for} \quad z \to \infty$$
(83)

$$\frac{l_h}{l_m} = 1 \qquad \text{for} \quad z = 0 \tag{84}$$

The second relation is always true. We will keep the 'old' values for λ_m and β_m and modify the ratios $\frac{\lambda_h}{\lambda_m}$ and $\frac{\beta_h}{\beta_m}$ so, that the condition (83) will be met. At this time we will use $\frac{\lambda_h}{\lambda_m} = C_{3free}$ and $\frac{\beta_h}{\beta_m} = 1$. In ACHMT is $C_3 = 1$.

2.6.2 Tuning parameter C_4

At this time we put $C_4 = 2.0$. We assume, that this value is good above the PBL ($C_3 = C_{3 free}$), but we will nead to tune C_4 near the surface.

Modification in antifibrilation scheme 2.7

Vertical exchange coefficients K_m and K_h are used in nonlinear vertical diffusion equation for computation of turbulent tendencies:

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left(K_{\psi} \frac{\partial \psi}{\partial z} \right)$$
(85)

where ψ stands for varibles u, v, θ, q .

Stiffness in this scheme can lead to spurious short-time but bounded oscillations-(termed "fibrilations") [1]. An antifibrilation scheme is used to eliminate this problem.

The principle of the 'antifibrilation' schemes is to time discretize the diffusion equation into a time-shifted formulation:[1]

$$\frac{\partial \psi}{\partial t} = \frac{\psi^+ - \psi}{\Delta t} = \frac{\partial \left[(1 - \beta) (K_\psi \frac{\partial \psi}{\partial z}) + \beta (K_\psi \frac{\partial \psi^+}{\partial z}) \right]}{\partial z}$$
(86)

where the superscript + represents the next time step, Δt is the physical time step length of the model, and β is the decentering factor.

The goal of the AF schemes is to locally determine β from the characteristics of the flow in order to ensure the stability of the scheme on the basis of a local linear stability analysis.[1]

In 'new' ACCOEFK and ACHMT we use the 'new' stability functions for calculations of environmental variables $K_m(11)$, $K_h(12)$ and α_u , α_θ :

$$\alpha_u = \frac{Ri}{F_m(Ri)} \left(\frac{dF_m(Ri)}{dRi} \right)$$
(87)

$$= Ri \left(\frac{d \ln(\sqrt{f(Ri)})}{dRi} \right)$$

$$= \frac{Ri}{2f(Ri)} \left(\frac{d f(Ri)}{dRi} \right)$$

$$= \frac{Ri}{Ri} \left(\frac{dF_h(Ri)}{dRi} \right)$$
(88)
(89)

$$\alpha_{\theta} = \frac{Ri}{F_h(Ri)} \left(\frac{dF_h(Ri)}{dRi} \right)$$
(89)

$$= Ri\left(\frac{d\ln(\sqrt{f(Ri)}\phi_3(Ri))}{dRi}\right) = Ri\left(\frac{d\ln(\frac{f(Ri)^2}{f(Ri)+C_4Ri})}{dRi}\right)$$
$$= \frac{3Ri}{2f(Ri)}\left(\frac{df(Ri)}{dRi}\right) - \frac{Ri}{f(Ri)+C_4}\left(\frac{df(Ri)}{dRi} + C_4\right)$$
(90)

where:

$$\frac{d f(Ri)}{dRi} = -(C_3 + C_4) + \frac{4C_4 - 2(C_3 + C_4)[1 - (C_3 + C_4)Ri]}{2\sqrt{(1 - (C_3 + C_4)Ri)^2 + 4C_4Ri}}$$
(91)

2.8 Current status

I started to work on this topic during my stay in Prague (4.06.2007 - 29.06.2007). At this time, the theoretical part is finished. Also some modifications in ACCOEFK subroutine code has been done. To make validation of 'new' ACCOEFK subroutine it is required to make new evaluation of the Prandtl-type mixing length from the TKE mixing length. Validation should be done together with new Prandtl-type mixing lengths when available.

2.9 Appendix

In the equation (40) was used following relation:

$$1 - RiC_3\phi_3(Ri) = f(Ri) \tag{92}$$

We will prove, that this relation is valid. Left side:

$$1 - RiC_3\phi_3(Ri) = 1 - \frac{C_3Rif(Ri)}{f(Ri) + C_4Ri} = \frac{f(Ri)\left(1 - C_3Ri\right) + C_4Ri}{f(Ri) + C_4Ri}$$
(93)

We need that:

$$f(Ri) (1 - C_3 Ri) + C_4 Ri = f(Ri)(f(Ri) + C_4 Ri)$$
(94)

We rewrite the right side of the relation (94):

$$f(Ri)(f(Ri) + C_4Ri) = f(Ri)f(Ri) + f(Ri)C_4Ri$$
 (95)

$$= 0.25 \left(X + \sqrt{X + 4C_4Ri} \right)^2 + 0.5 \left(X + \sqrt{X + 4C_4Ri} \right) C_4Ri \quad (96)$$

$$= 0.25 \left(X^{2} + 2X \sqrt{...} + \left(\sqrt{...} \right)^{2} \right) + 0.5C_{4}Ri \sqrt{...} + 0.5C_{4}RiX \quad (97)$$

$$= 0.25(2X^{2} + 4C_{4}Ri) + 0.5(X + C_{4}Ri)\sqrt{...} + 0.5C_{4}RiX$$
(98)
0.5 V(X + C_{4}Ri) + 0.5(X + C_{4}Ri)\sqrt{...} + 0.5C_{4}RiX (98)

$$= 0.5X(X + C_4Ri) + 0.5(X + C_4Ri)\sqrt{... + C_4Ri}$$
(99)

$$= 0.5(X + \sqrt{...})(X + C_4 Ri) + C_4 Ri$$
(100)
$$f(Ri)(1 - (C_4 + C_4)Ri + C_4 Ri) + C_4 Ri$$
(101)

$$= f(Ri)(1 - (C_3 + C_4)Ri + C_4Ri) + C_4Ri$$
(101)

$$= f(Ri)(1 - C_3Ri) + C_4Ri$$
(102)

where X is defined in relation (53).

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