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Examples of standard testcases used to benchmark oceanic vertical mixing parameterizations

Oceanic Boundary layer model

$$\begin{cases} \partial_t \mathbf{u}_h &= -f\mathbf{e}_z \times (\mathbf{u}_h - \mathbf{u}_g) + \partial_z \left(K_m \partial_z \mathbf{u}_h \right) - \mathcal{P}_x \mathbf{e}_x \\ \partial_t T &= \partial_z \left(K_s \partial_z T - \hat{\gamma} \right) + \dfrac{1}{\rho_0 C_p} \left[-\partial_z Q_s \right] \\ \partial_t S &= \partial_z \left(K_s \partial_z S - \hat{\gamma} \right) \end{cases}$$

with boundary conditions

$$K_m \partial_z \mathbf{u}_h(t)\big|_{z=0} = \boldsymbol{\tau}(t)/\rho_0 \qquad K_m \partial_z \mathbf{u}_h(t)\big|_{z=-H} = r_D \mathbf{u}_h(z=-H,t)$$

$$K_s \partial_z T(t)\big|_{z=0} = -\frac{1}{\rho_0 C_p}\left(Q_0(t) - Q_s^{\downarrow} \right) \qquad K_s \partial_z S(t)\big|_{z=0} = -S(z=0,t)(E-P)$$

$$\partial_z T(t)\big|_{z=-H} = \Gamma_T, \qquad \partial_z S(t)\big|_{z=-H} = \Gamma_S, \qquad Q_s(t)\big|_{z=0} = Q_s^{\downarrow}$$

Turbulent viscosity/diffusivity and the non-local term $\hat{\gamma}$ are given by

- 0-equation KPP closure scheme (KPP94 or KPP05)
- 1-equation TKE implementation (NEMO)
- 2-equation GLS closure scheme

Wind-induced deepening of boundary layer

Kato & Phillips : ***On the penetration of a turbulent layer into stratified fluid*, J. Fluid Mech., 1969**
Price : ***On the scaling of stress-driven entrainment experiments*, J. Fluid Mech., 1979**

- Parameters : $H = 50$ m, $T_0 = 16\ ^0$C, $\alpha = 2 \times 10^{-4}\ {}^o\text{C}^{-1}$, $N_0 = 0.01\ \text{s}^{-1}$
- Initial conditions :

$$S(z,0) = 35 \text{ psu}, \quad T(z,0) = T_0 - N_0^2(\alpha g)^{-1}|z|, \quad u(z,0) = v(z,0) = 0 \text{ m s}^{-1}$$

- Surface forcings ($u_\star^s = 0.01 \text{ m s}^{-1}$)

$$\tau_x(t)/\rho_0 = (u_\star^s)^2, \quad \tau_y = 0, \quad Q_0(t) = 0, \quad Q_s^{\downarrow}(t) = 0, \quad S(E-P)(t) = 0$$

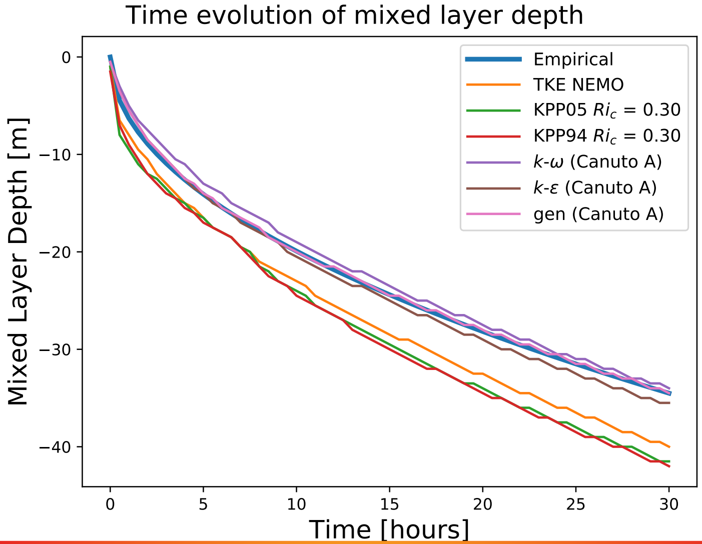
Relevant parameter to evaluate the simulations :

$\rightarrow$ Temporal evolution of mixed layer depth (Price, 1979)

$$D_{\text{ml}}(t) = 1.05 u_\star^s \sqrt{t/N_0}$$

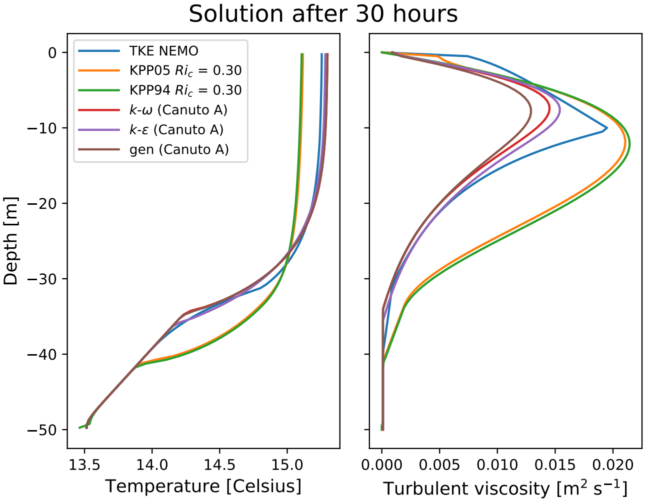
Wind-induced deepening of boundary layer

Numerical results ($\Delta t = 30$ s, $N = 100$ levels)



Wind-induced deepening of boundary layer

Numerical results ($\Delta t = 30$ s, $N = 100$ levels)



Free-convection simulation with constant cooling

Willis & Deardorff : *A laboratory model of the unstable planetary boundary layer*, J.A.S., 1974

Mironov et al.: *Vertical turbulence structure and second-moment budgets in convection with rotation: A Large-Eddy Simulation study*, QJRMS, 2000

- Parameters : $H = 50$ m, $\alpha = 2 \times 10^{-4}\ {}^{o}\mathrm{C}^{-1}$, $N_0 = \sqrt{\alpha g (0.1\ {}^{0}\mathrm{C}\ \mathrm{m}^{-1})}$
- Initial conditions :

$$S(z,0) = 35 \text{ psu}, \quad T(z,0) = T_0 - N_0^2 (\alpha g)^{-1} |z|, \quad u(z,0) = v(z,0) = 0 \text{ m s}^{-1}$$

- Surface forcings

$$\tau_x = \tau_y = 0, \quad Q_0(t) = -\frac{100}{\rho_0 C_p}, \quad Q_s^{\downarrow}(t) = 0, \quad S(E-P)(t) = 0$$

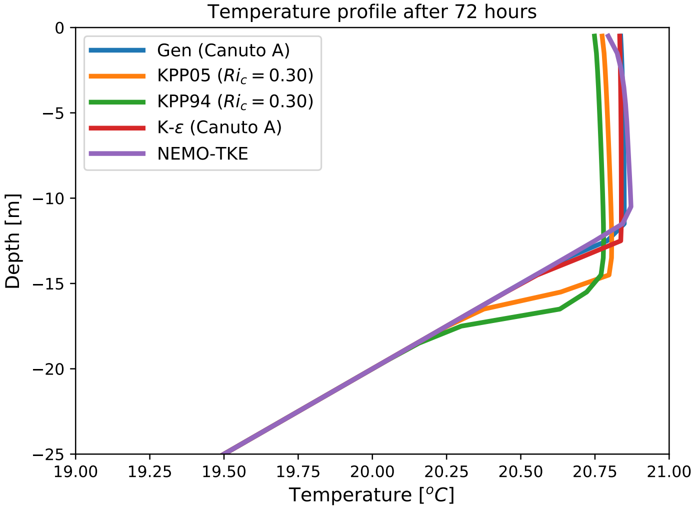
Relevant parameter to evaluate the simulations :

$\rightarrow$ LES study by Mironov et al. (2000) + theory by Zilitinkevich (1991)

Free-convection simulation with constant cooling

Numerical results

Theoretical depth of the boundary layer : $D_m \approx 11.6$ m (Zilitinkevich; 1991)



Turbulent Ekman bottom boundary layer

Andren et al. *Large-eddy simulation of a neutrally stratified boundary layer: A comparison of four computer codes*, QJRMS, 1994

- Parameters : $H = 1500$ m, $f = 10^{-4}$ s^{-1}, $z_{0,b} = 0.1$ m, $N = 40$ levels
- Initial conditions :

$$u(z,0) = u_G = 10 \text{ m s}^{-1}, \quad v(z,0) = v_G = 0 \text{ m s}^{-1}$$

- Bottom forcing

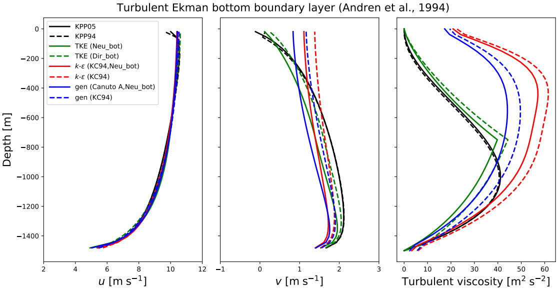
$$K_m \partial_z \mathbf{u}_h(t)|_{z=-H} = r_D \mathbf{u}_h(-H,t), \quad r_D = \|(\mathbf{u}_h)_1\| \left(\frac{\kappa}{\left(\frac{z_{0,b}}{\Delta z_1}+1\right)\ln\left(\frac{\Delta z_1}{z_{0,b}}+1\right)-1} \right)^2$$

Relevant parameter to evaluate the simulations :

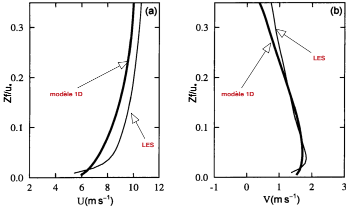
$\rightarrow$ LES reference solution

Turbulent Ekman bottom boundary layer

Numerical results



Cuxart et al., 2000



Pressure-gradient driven flow

- Parameters : $H = 5$ m, $N = 50$ levels, $z_{0,b} = 0.01$ m
- Simplified model

$$\partial_t u = \partial_z (K_m \partial_z u) - \mathcal{P}_x$$

- Bottom boundary condition

$$\tau_x / \rho_0 = u_{\star,b}^2 = \mathcal{P}_x H$$

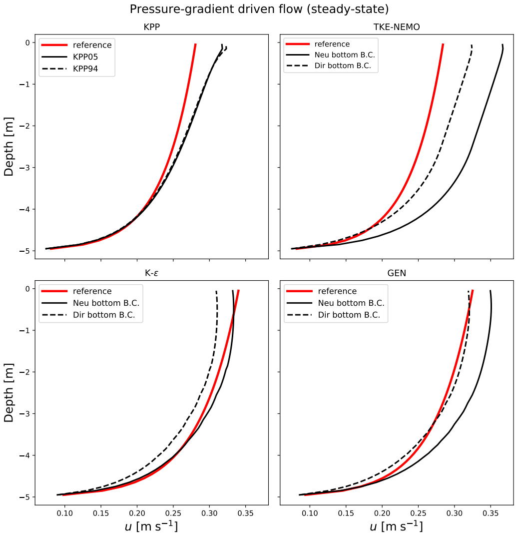
Relevant parameter to evaluate the simulations :

$\rightarrow$ steady state analytical profile

$$u(z) = \frac{\sqrt{\mathcal{P}_x H}}{\kappa} \ln \left(\frac{z + H + z_{0,b}}{z_{0,b}} \right), \qquad z \in [-H, 0]$$

Pressure-gradient driven flow

Numerical results



- ▷ KPP shape function follows MO theory
- ▷ Mixing length form in NEMO-TKE ignores MO theory

Going further in the evaluation of vertical mixing parameterizations

- Idealized testcases with analytical initial/boundary conditions and comparison with LES (ongoing work within the CVmix initiative)

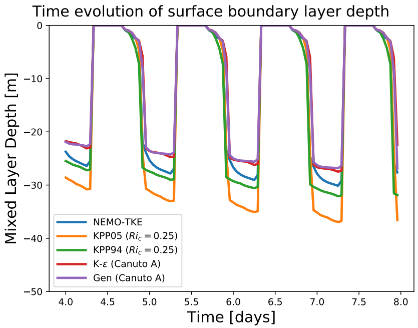
- Comparison with buoy measurements (e.g. PAPA station) or in situ microstructure measurements (e.g. Costa et al., 2017)

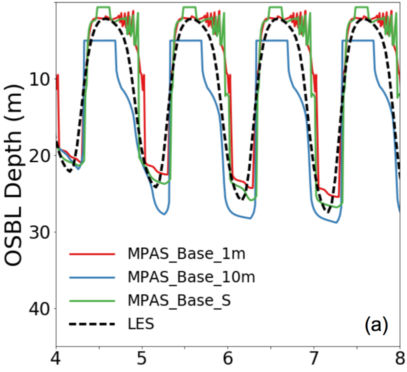
- Laboratory experiments ?

Testcase from CVmix community

Van Roekel et al. ***The KPP boundary layer scheme: revisiting its formulation and benchmarking one-dimensional ocean simulations relative to LES*****, in prep.**

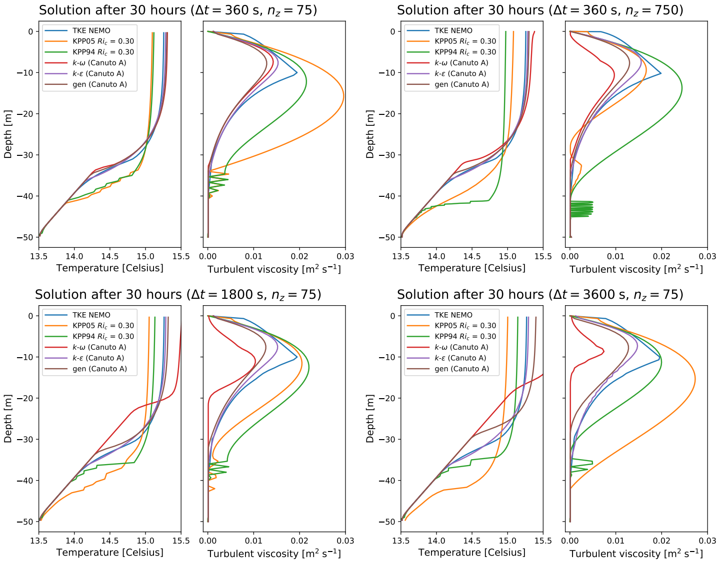
→ Same as Willis & Deardorff but with diurnal cycle





Van Roekel et al.

Δt and Δz dependency of numerical results



2

Space-time discretization issues

Positivity preservation for TKE and length scale/ε

Patankar *Numerical Heat Transfer and Fluid Flow*, 1980
Deleersnijder et al. *Some mathematical problems associated with the development and use of marine models*, 1997

$\rightarrow$ Discretised forms of the equations must retain the principle of non-negativity

$$\begin{cases} \partial_t \phi &= S - P\phi, \qquad S, P > 0 \\ \phi(t=0) &= \phi_0 > 0 \end{cases}$$

Example : Patankar procedure to ensure non-negativity of TKE

- If $S = K_m \left[(\partial_z u)^2 + (\partial_z v)^2 \right] - K_t N^2 > 0$

$$\mathrm{TKE}^{n+1} = \mathrm{TKE}^n + \Delta t \left[S - \left(\frac{c_\varepsilon}{L} \sqrt{\mathrm{TKE}^n} \right) \mathrm{TKE}^{n+1} \right]$$

- Otherwise

$$\mathrm{TKE}^{n+1} = \mathrm{TKE}^n + \Delta t \left[(S + K_t N^2) - \left(\frac{K_t N^2}{\mathrm{TKE}^n} + \frac{c_\varepsilon}{L} \sqrt{\mathrm{TKE}^n} \right) \mathrm{TKE}^{n+1} \right]$$

$\Rightarrow$ Extension to higher-order (Runge-Kutta) methods, see Kopecz & Meister (Appl Numer Math, 2017)

Energetic consistency – mixing terms vs turbulent closure

Burchard *Energy-conserving discretisation of turbulent shear and buoyancy production*, 2002
Marsaleix et al. *Energy conservation issues in σ-coordinate free-surface ocean models*, 2008

$$\begin{aligned} \partial_t u - \partial_z \left(K_m \partial_z u\right) &= 0 \\ \partial_t b - \partial_z \left(K_s \partial_z b\right) &= 0 \end{aligned} \quad \rightarrow \quad \begin{aligned} \partial_t \mathrm{KE} - \partial_z \left(K_m \partial_z \mathrm{KE}\right) &= -K_m \left(\partial_z u\right)^2 &= -P \\ \partial_t \mathrm{PE} - \partial_z \left((-z) K_s \partial_z b\right) &= K_s \;\; \partial_z b &= -B \end{aligned}$$

$$\partial_t \mathrm{TKE} - \partial_z \left(K_e \partial_z \mathrm{TKE}\right) = P + B - \varepsilon$$

Energy budget in a water column (ignoring the contribution of B.C.) :

$$E = \int_{-H}^{0} (\mathrm{KE} + \mathrm{PE} + \mathrm{TKE}) dz \qquad \rightarrow \qquad \partial_t E = -\int_{-H}^{0} \varepsilon dz$$

Same rationale can be applied in a discrete sense

For example for the shear term (on a C-grid) :

ad-hoc $$P_{i,k+1/2} = (K_m)_{i,k+1/2} \left[\left(\overline{(\partial_z u)_{k+1/2}}^{(i)} \right)^2 + \left(\overline{(\partial_z v)_{k+1/2}}^{(j)} \right)^2 \right]$$

E-conserving $$P_{i,k+1/2} = \overline{\overline{(K_m)_{k+1/2}}^{(i)} (\partial_z u)^2_{k+1/2}}^{(i)} + \overline{\overline{(K_m)_{k+1/2}}^{(j)} (\partial_z v)^2_{k+1/2}}^{(j)}$$

+ consistent time integration between $\partial_t \mathrm{TKE}$, $\partial_t \mathrm{KE}$ and $\partial_t \mathrm{PE}$

Parabolic Courant number in realistic simulations (1/3)

Lemarié et al. ***Stability Constraints for Oceanic Numerical Models: Implications for the Formulation of Time and Space Discretizations*****, Ocean Mod., 2015**

Exact damping rate ω^e for the diffusion equation with diffusivity κ :

$$\omega^e = \kappa k_z^2 = \frac{\sigma^{(2)}\theta^2}{\Delta t}, \qquad \sigma^{(2)} = \frac{\kappa \Delta t}{\Delta z^2}, \quad \theta = k_z \Delta z$$

numerical damping rate for a numerical scheme with amplification factor $\mathcal{A}$

$$\omega^{\text{num}} = -\log|\mathcal{A}(\sigma^{(2)}, \theta)|/\Delta t, \qquad \mathcal{A}^{\text{Euler}} = \left[1 + 2\sigma^{(2)}(1 - \cos\theta)\right]^{-1}$$

Effective diffusivity κ^{eff} which would account for numerical errors

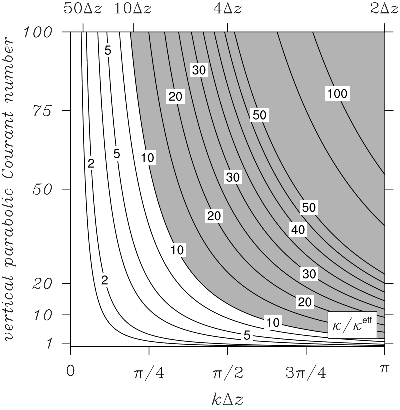
$$\omega^e = \kappa^{\text{eff}} k_z^2 \qquad \text{such that} \qquad \omega^e = \omega^{\text{num}}$$

$\rightarrow$ κ^{eff} is the diffusivity in the continuous equation which would give the same damping as the numerical damping

Parabolic Courant number in realistic simulations (2/3)

Lemarié et al. *Stability Constraints for Oceanic Numerical Models: Implications for the Formulation of Time and Space Discretizations*, Ocean Mod., 2015

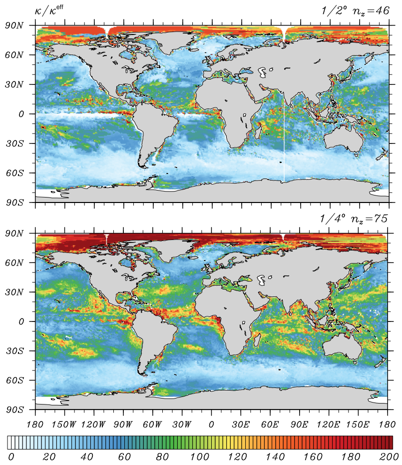
For backward Euler scheme



$\kappa/\kappa^{\rm eff} \gg 1 \Rightarrow$ the damping seen by the model is smaller than the theoretical damping associated to the diffusivity value κ.

Parabolic Courant number in realistic simulations (3/3)

Lemarié et al. *Stability Constraints for Oceanic Numerical Models: Implications for the Formulation of Time and Space Discretizations*, Ocean Mod., 2015



$$
\begin{aligned}
\sigma^{(2)} &= \overline{\sigma}^{(\mathrm{mld})} \\
\theta &= 2\pi/N_{\mathrm{mld}}
\end{aligned}
$$

Space-time discretization of physical parameterizations is often overlooked (with the possibility to compromise the physical principles)

Delicacies associated with nonlinear vertical diffusion

Deleersnijder et al. *On the mathematical stability of stratified flow models with local turbulence closure schemes*, 2008

The eddy coefficients are not independent of the gradient of the solution

$$\left\langle w'\phi' \right\rangle = -K_z \partial_z \phi \qquad \longrightarrow \qquad \partial_t \phi = \partial_z \left(K_z \partial_z \phi \right)$$

Let us assume that $K_z(\phi, z) = (\partial_z \phi)^{-2}$

- $K_z > 0 \qquad \rightarrow$ well-behaved solution ?

$$\partial_z \phi_z = \partial_z \left(\widetilde{K_z} \partial_z \phi_z \right), \qquad \phi_z = \partial_z \phi, \qquad \widetilde{K_z} = -\left(\partial_z \phi \right)^{-2}$$

- $\widetilde{K_z} < 0 \quad \rightarrow$ gradient can grow unbounded while ϕ would remain bounded

"fibrillations" associated with nonlinear vertical diffusion

At a discrete level, the use of a simple Euler backward scheme

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \partial_z \left(K_z(\phi^{n}) \partial_z \phi^{n+1} \right)$$

does not guarantee stability in a nonlinear sense (e.g. Kalnay & Kanamitsu 1988).

Various alternatives proposed, mostly based on the following model problem

$$\partial_t \phi = -(K \phi^P) \phi + S, \qquad K_z \approx K \phi^P$$

- Girard & Delage, *Stable schemes for nonlinear vertical diffusion in atmospheric circulation models*, MWR, 1990
- Benard, *Stabilization of nonlinear vertical diffusion schemes in the context of NWP Models*, MWR, 2000
- Wood et al., *A monotonically-damping second-order-accurate unconditionally-stable numerical scheme for diffusion*, QJRMS, 2007
- Nazari et al., *A stable and accurate scheme for nonlinear diffusion equations: Application to atmospheric boundary layer*, JCP, 2013

$\Rightarrow$ This issue is absent from oceanic literature ...
because of parameterization formulation or $\neq$ physical time-scales in BL ?