

Column models and large eddy simulation of the ocean surface boundary layer

Greg, Andre, Raf

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1 Introduction

Turbulence persists throughout Earth's ocean, but nowhere is it more vigorous than in the surface boundary layer. In the ocean surface boundary layer, or the 'OSBL', a gallimaufry of phenomena — surface cooling and heating, precipitation and evaporation, propagating and breaking surface waves, sheared currents and propagating internal waves, atmospheric turbulence and steady winds — drive turbulence and turbulent mixing that transfers heat, salinity, carbon, and momentum from the atmosphere into the ocean interior.

1.1 Fluxes, stresses, and turbulence

The depth to which surface-driven turbulence penetrates is limited by the time-dependence and finite intensity of the atmospheric forcing, and the potential energy that must be created to erode the typically strongly stable stratification of the interior ocean. Accurately predicting the depth of the turbulent surface 'mixing layer' as a function of momentum and buoyancy fluxes is one of the primary tasks of a surface boundary layer model.

We entertain a radically simplified view of boundary layer dynamics in which turbulence in the surface boundary layer is driven by

1. Momentum flux, $\mathbf{F}_u = F_u \hat{\mathbf{x}} + F_v \hat{\mathbf{y}}$, associated with atmospheric winds and waves, and
2. Buoyancy flux, F_b , associated with latent and sensible heating, precipitation, and radiation.

We define flux in the sense ordinary to physics: a *positive* flux implies an upward flux of a given quantity. In consequence, a positive buoyancy flux acts to *reduce* the buoyancy of the ocean beneath (because buoyancy is sucked upward, out of the ocean); therefore positive buoyancy flux is *destabilizing* and leads to convection. The same relationship holds for the effects of \mathbf{F}_u on horizontal momentum U and V .

We refer to the oceanographic quantity Q (often confusingly called surface heat flux) as 'heating'; so that, logically, $Q < 0$ implies cooling of the ocean surface boundary layer. If latent and sensible heating dominate buoyancy fluxes, then

$$F_b = -\frac{\alpha g Q}{\rho_0 c_P}, \quad (1)$$

where ρ_0 is some density, c_P is some representative heat capacity for the ocean surface layer, and α is the thermal expansion coefficient that relates changes in temperature to changes in fluid density and therefore buoyancy. Similarly, the relationship between 'wind stress' $\boldsymbol{\tau}$ and momentum flux \mathbf{F}_u is

$$\mathbf{F}_u = -\frac{\boldsymbol{\tau}}{\rho_0}. \quad (2)$$

1.2 Characteristic velocity scales of boundary layer turbulence

The characteristic turbulent velocity scale associated with convection (Deardorff, 1972) is

$$\varpi_b \stackrel{\text{def}}{=} |hF_b|^{1/3} . \quad (3)$$

Note that when $F_b < 0$, the buoyancy forcing is stable and convection does not occur. In this case a non-zero ϖ_b is dubious and perhaps should not be used. We include this quantity here despite the possibility for confusion because of its use in standard KPP.

The characteristic turbulent velocity scale associated with wind stress is the friction velocity

$$\varpi_\tau \stackrel{\text{def}}{=} \left| \frac{\boldsymbol{\tau}}{\rho_0} \right|^{1/2} = \frac{\sqrt{\tau_u^2 + \tau_v^2}}{\rho_0} . \quad (4)$$

An idea implicit in KPP is a *composite* turbulent vertical scale associated with the combination of buoyancy flux and wind-driven mixing. However, unlike the vertical scales for pure convection and pure wind mixing, this composite scale cannot be expressed as a scalar in KPP; instead, it is a complicated function of depth. A possible simplification of KPP would separate the concept of a composite turbulent vertical scale from the depth dependence of the turbulent diffusivity.

2 The K-Profile-Parameterization

The K-Profile-Parameterization, known colloquially as ‘KPP’, is a parameterization for subgrid vertical turbulent fluxes of scalars and momentum in the ocean’s surface boundary layer. We decompose exact fields into $\phi = \Phi + \phi'$, where $\Phi \stackrel{\text{def}}{=} \bar{\phi}$ is a horizontally-averaged, slowly-varying part of ϕ , and ϕ' its subgrid counterpart. KPP parameterizes the subgrid vertical turbulent flux $\overline{w'\phi} - W\Phi \approx \overline{w'\phi'}$ as

$$\overline{w'\phi'} = -K_\Phi \partial_z \Phi + N_\Phi , \quad (5)$$

where K_Φ is a turbulent diffusivity and F_N is a non-local vertical flux associated with surface fluxes of Φ .

The large-scale temperature evolution equation, for example, is then

$$\partial_t T + \mathbf{U} \cdot \nabla T = \kappa_T \Delta T + \partial_z (K_T \partial_z T - N_T) + I_T , \quad (6)$$

where κ_T is the molecular diffusivity of temperature and I_T represents an internal source of temperature associated, for example, with solar insolation. The evolution equation for momentum, on the other hand, is

$$\partial_t \mathbf{U} + (\mathbf{U} \cdot \nabla) \mathbf{U} + \mathbf{f} \times \mathbf{U} = -\nabla P + \nu \Delta \mathbf{U} + \partial_z (K_U \partial_z \mathbf{U}) . \quad (7)$$

There is no non-local flux for momentum.

To describe KPP, we denote ‘model parameters’ — scalar values chosen so the model ‘fits’ the data — as $C_{\text{var}}^{\text{label}}$, where ‘label’ is intended to identify and describe the parameter and ‘var’ is the variable: U , V , T , S , or the catch-all Φ , to which it refers. We denote ‘model functions’ as $\Upsilon_{\text{var}}^{\text{label}}$ with the same logic.

2.1 Key elements of KPP

Three basic elements comprise the K-Profile-Parameterization:

1. A definition of the ‘mixing depth’ h , the depth to which unresolved boundary layer turbulence penetrates, and thus the depth over which turbulence driven by surface forcing acts to mix oceanic quantities. h is called the ‘mixed layer depth’ or ‘boundary layer depth’ in Large *et al.* (1994). Yet in some scenarios — especially those with strong transients or without strong surface forcing — h may

differ significantly from the depth of a well-mixed layer of resolved variables. In KPP, h is defined as a function of the surface buoyancy flux F_b , the resolved buoyancy field B , the resolved boundary layer potential energy PE, and resolved boundary layer kinetic energy KE:

$$h = \Upsilon^h(\text{PE}, \text{KE}, F_b, B). \quad (8)$$

In most implementations of KPP the function Υ^h is implicit. The definition of PE and KE is part of the KPP model and differs between implementations.

2. A definition of the boundary layer eddy diffusivity, K_Φ , for a variable Φ . Φ may be horizontal velocity, temperature, salinity, or other passive tracers. In KPP, the depth-varying, variable-dependent boundary layer eddy diffusivity is a function of boundary layer depth h , surface buoyancy flux, and surface momentum flux $\mathbf{F}_u = F_U \hat{\mathbf{x}} + F_V \hat{\mathbf{y}}$:

$$K_\Phi = \Upsilon_\Phi^{\text{diffusivity}}(\mathbf{F}_u, F_b, h). \quad (9)$$

3. A definition of ‘non-local’ fluxes for *tracers*

$$N_\Phi = \Upsilon_\Phi^{\text{non-local}}(F_\Phi, h), \quad (10)$$

in terms of surface fluxes F_Φ and boundary layer depth h . There is no non-local flux for momentum in KPP.

In addition to these three main components, the concept of a two-part boundary layer is embedded in KPP. The upper part of the boundary layer is the ‘surface layer’, which extends to some fraction C^ϵ of the total boundary layer depth h . C^ϵ is a model constant which is typically taken to be 0.1.

2.2 Non-local flux

The non-local flux is

$$N_\Phi = C^N \Upsilon^N(d) F_\Phi, \quad (11)$$

where F_Φ is the surface flux of a quantity Φ , $C^N = 6.33$ is a model parameter, and $\Upsilon^N(d)$ is a non-dimensional shape function that distributes the surface flux over the boundary layer depth h as a function of the non-dimensional depth $d = -z/h$:

$$\Upsilon^N(d) \stackrel{\text{def}}{=} d(1-d)^2. \quad (12)$$

$\Upsilon^N(d)$ in (12) ensures that the non-local flux vanishes at the surface and bottom of the mixing layer.

2.3 Local diffusivity

The local diffusivity K_Φ of a quantity Φ is formulated with a mixing-length argument, so that

$$K_\Phi \propto \text{length} \times \text{velocity scale}, \quad (13)$$

where the length is the boundary layer depth h and the velocity scale is a depth-dependent function of the wind stress and surface buoyancy flux. As a function of the non-dimensional depth $d = -z/h$, K_Φ is

$$K_\Phi(d) \stackrel{\text{def}}{=} h \Upsilon_\Phi^w(d) \Upsilon^K(d), \quad (14)$$

where $\Upsilon^K(d)$ in (14) is the state-independent shape function:

$$\Upsilon^K(d) = d(1-d)^2. \quad (15)$$

The function $\Upsilon_{\Phi}^w(d)$ in (14), with units of velocity, models the depth dependence of the velocity scale of turbulent mixing associated with the interaction of wind stress and convection. The model assumes that there are two distinct turbulence regimes associated with convection due to destabilizing buoyancy flux $F_b > 0$ or due to the interaction between wind-driven mixing and a stabilizing buoyancy flux, $F_b < 0$. With a stabilizing buoyancy flux and no wind, $\Upsilon_{\Phi}^w \rightarrow 0$.

2.3.1 Limiting cases: local diffusivities in pure convection or pure wind mixing

The turbulent vertical velocity scale in boundary layers driven purely by wind mixing is

$$\Upsilon_{\Phi}^w(d) = C^{\kappa} \varpi_{\tau}, \quad (16)$$

where $C^{\kappa} = 0.4$ is interpreted as the ‘Von Karman constant’. The diffusivity profile in pure wind mixing is therefore

$$K_{\Phi}(d) = C^{\kappa} h \varpi_{\tau} d(1-d)^2, \quad (17)$$

for all velocity fields and tracers.

The turbulent vertical velocity scale in pure convection is different for momentum than it is for tracers, though their functional forms are the same. Both functions are formulated in terms of a ‘truncated’ non-dimensional depth $d_{\epsilon} = \min(C^{\epsilon}, d)$:

$$\Upsilon_{\Phi}^w(d_{\epsilon}) = \varpi_b (C_{\Phi}^b d_{\epsilon})^{1/3}. \quad (18)$$

The constants for momentum and tracers that factor in (18) are $C_U^b = 0.215$ and $C_T^b = 2.53$, respectively. These constants imply the turbulent, pure-convection turbulent Prandtl number is

$$Pr^{\text{turb}} \stackrel{\text{def}}{=} \frac{K_U}{K_T} = \left(\frac{C_U^b}{C_T^b} \right)^{1/3} = 0.440, \quad (19)$$

below the surface layer where $d > C^{\epsilon}$. The diffusivities under pure convection in the upper surface layer where $d < C^{\epsilon}$ are $K_{\Phi} = h \varpi_b (d C_{\Phi}^b)^{1/3} d(1-d)^2$, and below are

$$K_{\Phi}(d) = (C^{\epsilon} C_{\Phi}^b)^{1/3} h \varpi_b d(1-d)^2. \quad (20)$$

Note that with $C^{\epsilon} = 0.1$ we have $(C^{\epsilon} C_U^b)^{1/3} = 0.278$ and $(C^{\epsilon} C_T^b)^{1/3} = 0.632$.

2.3.2 The vertical velocity scale in stable, wind-mixed boundary layers

In KPP, a stabilizing buoyancy flux divides (16) by $1 + C^{\tau b} \left(\frac{\varpi_b}{\varpi_{\tau}} \right)^3 d = 1 + C^{\tau b} \left(\frac{h|F_b|}{|\tau/\rho_0|^{3/2}} \right) d$, where $C^{\tau b} = 5C^{\kappa} = 2.0$, thereby reducing the wind-driven turbulent diffusivity for momentum and tracers alike. The resulting turbulent vertical velocity scale due the combination of wind-driven mixing and a stabilizing buoyancy flux is

$$\Upsilon_{\Phi}^w(d) = C^{\kappa} \frac{\varpi_{\tau}}{1 + C^{\tau b} \left(\frac{\varpi_b}{\varpi_{\tau}} \right)^3 d}. \quad (21)$$

Note that the concept of a turbulent vertical velocity scale associated with stable buoyancy forcing is clearly invalid. It is unclear whether the ratio $\left(\frac{\varpi_b}{\varpi_{\tau}} \right)^3 = \frac{h|F_b|}{|\tau/\rho_0|^{3/2}}$ is appropriate to use in this case.

2.3.3 The vertical velocity scale in unstable, convecting, and wind-mixed boundary layers

The effect of wind mixing on the turbulent vertical velocity scale in unstable convecting boundary layers is complex. In addition to the facts that, as in convecting boundary layers without wind stress,

1. the vertical velocity scales are *different* for the velocities U and V than for scalars like T and S , so that $\Upsilon_U^w \neq \Upsilon_T^w$; and
2. the dependence of the vertical velocity on depth is confined to the surface layer where $0 < d < C_\epsilon$,

we confront the additional layer of complication that

3. the unstable vertical velocity scale is a piecewise function that changes form around a critical value of $(\varpi_\tau/\varpi_b)^3 d$.

To simplify the presentation, we define a ‘scaled depth’ $\tilde{d} = (\varpi_b/\varpi_\tau)^3 d$ and a ‘truncated scaled depth’, $\tilde{d}_\epsilon = (\varpi_b/\varpi_\tau)^3 \min[d, \epsilon]$. The unstable turbulent velocity scale then changes character around $\tilde{d}_\epsilon = 0.5$ for momentum and $\tilde{d}_\epsilon = 2.5$ for tracers. This change in behavior is intended to capture a distinction between regimes of ‘strong’ and ‘weak’ wind effect on convective turbulence, since \tilde{d} decreases as wind stress increases.

In terms of the truncated scaled depth, the turbulent vertical velocity scale functions are

$$\Upsilon_\Phi^w(\tilde{d}_\epsilon) = \begin{cases} \varpi_\tau (C_\Phi^{\tau+} + C_\Phi^{b+} \tilde{d}_\epsilon)^{n_\Phi} & \text{for } C_\Phi^d \geq \tilde{d}_\epsilon \geq 0, \\ \varpi_\tau (C_\Phi^\tau + C_\Phi^b \tilde{d}_\epsilon)^{1/3} & \text{for } \tilde{d}_\epsilon > C_\Phi^d. \end{cases} \quad (22)$$

where the function exponent in the ‘wind-dominated regime’ is $n_U = 1/4$ for momentum and $n_T = 1/2$ for tracers. The transitional depth constants are $C_U^d = 0.5$ for momentum and $C_T^d = 2.5$ for tracers.

The shallow ‘+’ functional forms significantly modify the vertical velocity scale when wind mixing is relatively strong compared to convection, especially for tracers. At the bottom of the surface layer where $d = C_\epsilon$, the piecewise functional form transitions between behaviors around the critical forcing ratio $\varpi_\tau/\varpi_b = (C_\epsilon/C_\Phi^d)^{1/3} = 0.585$ or 0.312 for momentum or tracers, respectively.

The 6 new model constants introduced in the functions in (22) are

$$C_U^{\tau+} = \kappa^4 \quad (23)$$

$$C_U^{b+} = 16\kappa^5 \quad (24)$$

$$C_T^{\tau+} = \kappa^2 \quad (25)$$

$$C_T^{b+} = 16\kappa^3 \quad (26)$$

$$C_U^\tau = 1.26\kappa^3 \quad (27)$$

$$C_T^\tau = -28.86\kappa^3 \quad (28)$$

and $C_U^b = 0.215$ and $C_T^b = 2.53$ are defined previously.

Note that in the limit of zero wind where $\varpi_\tau \rightarrow 0$, the thickness wind-dominated layer shrinks to 0, leaving only the lower layer formula, which itself then limits to (18).

2.4 Diagnosis of boundary layer depth

The boundary layer depth h is defined implicitly via the Richardson criterion,

$$C^{\text{Ri}} = \frac{h\Delta B}{|\Delta U|^2 + \Upsilon^{KE}}, \quad (29)$$

where the boundary layer differential of a resolved quantity Φ is defined as a function of h by

$$\Delta\Phi(-h) \stackrel{\text{def}}{=} \frac{1}{C^\epsilon h} \int_{-C^\epsilon h}^0 \Phi dz - \Phi(-h). \quad (30)$$

$\Delta\Phi(-h)$ is the difference between the ‘surface layer’ average of Φ and its value at $z = -h$. The model constant $C^{\text{Ri}} = 0.3$ in (29) represents the fractional amount of kinetic energy $\Upsilon^{\text{KE}} + |\Delta\mathbf{U}|^2$ that must accumulate in order to overturn the boundary layer potential energy, $h\Delta B$. We are using the Richardson number definition proposed by Van Roekel *et al.* (2018), hereafter VR18.

The function $\Upsilon^{\text{KE}}(-h)$ in (29) parameterizes ‘unresolved turbulent kinetic energy’ due to convective activity, and is defined

$$\Upsilon^{\text{KE}}(-h) = C^{\text{KE}} h^{4/3} \sqrt{\max[0, B_z(-h)]} \max[0, F_b^{1/3}], \quad (31)$$

where $C^{\text{KE}} = C^V \sqrt{0.2}/C^{\text{Ri}} C^\kappa (98.96 C^\epsilon)^{1/6} = 4.32$ with $C^V = 1.7$ a model constant. When $F_b > 0$, (31) becomes

$$\Upsilon^{\text{KE}}(-h) = \frac{C^{\text{KE}}}{C^V} h N_e \varpi_b, \quad (32)$$

where $N_e^2 \stackrel{\text{def}}{=} B_z(-h)$ is the buoyancy gradient at the ‘entrainment depth’. The factor C^V , which is not an independent constant in our formulation, is intended to account for the difference between the buoyancy gradient at the entrainment depth and h .

A Connections with Large *et al.* (1994)

In Large *et al.* (1994), the vertical velocity scale is formulated in terms of ‘stability functions’ Υ_ϕ^s , so that

$$\Upsilon_\phi^w = \frac{C^\kappa \varpi_\tau}{\Upsilon_\phi^s(\zeta)}, \quad (33)$$

where ζ is a depth-like similarity variable defined by

$$\zeta \stackrel{\text{def}}{=} -\frac{z}{L}, \quad (34)$$

$$= -C^\kappa \left(\frac{\varpi_b}{\varpi_\tau} \right)^3 d, \quad (35)$$

where $L = -\varpi_\tau^3/C^\kappa F_b = -h\varpi_\tau^3/C^\kappa \varpi_b^3$ is the ‘Monin-Obukhov length’. In this document, we work with the slightly different variable

$$\tilde{d} \stackrel{\text{def}}{=} \left(\frac{\varpi_b}{\varpi_\tau} \right)^3 d = -\frac{\zeta}{C^\kappa}. \quad (36)$$

This variable is preferred because it does not include the model parameter C^κ . The stability functions have the property $\Upsilon_\phi^s(0) = 1$, so that in pure wind mixing, where $F_b = \varpi_b = L = 0$, the vertical velocity scale is $\Upsilon_\phi^w = C^\kappa \varpi_\tau$.

B Model parameters and model functions

Model parameters are denoted C and model function are denoted Υ . The model parameters defined by KPP are

The model functions defined by KPP are

Table 1: Model parameters in KPP. UBLs are convecting, 'Unstable Boundary Layers'.

Param	Value	Formula and reference	Description
C^ϵ	0.100	CVMix (8.127)	Surface layer fraction
C^N	6.33	$C_* C^\kappa (c_s C^\kappa C^\epsilon)^{1/3}$ CVMix (8.141)	Non-local flux proportionality
C^κ	0.400	LMD94 eq 2	Von Karman constant
$C^{\tau b}$	2.00	$5C^\kappa$, LMD94 eq 2, 13, B1a	$\Upsilon_\phi^w(d)$ reduction for stabilizing F_b
C_U^b	0.215	$8.38 (C^\kappa)^4$, LMD94 eq 2, 13, B1c, B2	Convection factor for $\Upsilon_U^w(d)$
C_T^b	2.53	$98.96 (C^\kappa)^4$, LMD94 eq 2, 13, B1e, B2	Convection factor for $\Upsilon_T^w(d)$
C_U^τ	0.0806	$1.26 (C^\kappa)^3$ from LMD94 2, 13, B1c, B2	Effect of wind mixing on $\Upsilon_U^w(d)$ in UBLs
C_T^τ	-1.85	$-28.86 (C^\kappa)^3$ from LMD94 2, 13, B1b	Effect of wind mixing on $\Upsilon_T^w(d)$ in UBLs
$C_U^{\tau+}$	0.0256	$(C^\kappa)^4$ from LMD94 2, 13, B1b	Effect of wind mixing on upper $\Upsilon_U^w(d)$ in UBLs
C_U^{b+}	0.164	$16 (C^\kappa)^5$ from LMD94 2, 13, B1b	Upper layer convection factor for $\Upsilon_U^w(d)$
$C_T^{\tau+}$	0.160	$(C^\kappa)^2$ from LMD94 2, 13, B1d	Effect of wind mixing on upper $\Upsilon_T^w(d)$ in UBLs
C_T^{b+}	1.02	$16 (C^\kappa)^3$ from LMD94 2, 13, B1d	Upper layer convection factor for $\Upsilon_T^w(d)$
C^{KE}	4.32	$\sqrt{0.2} C_v / C^{Ri} C^\kappa (98.96 C^\epsilon)^{1/6}$, CVMix §8.5.7.4	Unresolved convective kinetic energy
C^{Ri}	0.300	CVMix eq 8.187	Bulk Richardson number criterion

Table 2: Model functions in KPP.

Model function	Value	Units	Description
$\Upsilon^K(d)$	$d(1-d)^2$	none	Shape function for effective diffusivity
$\Upsilon^N(d)$	$d(1-d)^2$	none	Shape function for non-local flux
$\Upsilon_\phi^w(d)$	eq (12)	m s^{-1}	Turbulent velocity scale
$\Upsilon^{KE}(h)$	eq (15)	$\text{m}^2 \text{s}^{-2}$	Convective turbulent kinetic energy function

Table 3: Notation in this document.

Variable	Description
K_Φ	Effective subgrid diffusivity of quantity Φ
N_Φ	Non-local subgrid flux of quantity Φ
F_Φ	Surface flux of quantity Φ
F_b	Surface buoyancy flux
τ	Wind stress
$\varpi_\tau = \tau/\rho_0 ^{1/2}$	Turbulent velocity scale for wind mixing
$\varpi_b = (hF_b)^{1/3}$	Turbulent velocity scale for convection
h	Boundary layer depth
$d = -z/h$	Non-dimensional boundary layer depth coordinate
$\tilde{d} = (\varpi_\tau/\varpi_b)^3 d$	Surface-flux-scaled boundary layer depth coordinate

C Simple cases and tests for KPP

Consider a temperature profile $T(z) = T_0 + \gamma z$. In the case that $C^\epsilon \rightarrow 0$, find that

$$\Delta B(-h) \approx B(0) - B(-h), \quad (37)$$

$$= g\alpha\gamma h. \quad (38)$$

For $h > 0$ we further have $B_z = g\alpha\gamma$, and

$$\gamma^{\text{KE}}(-h) = C^{\text{KE}} h^{4/3} \sqrt{g\alpha\gamma} F_b^{1/3}. \quad (39)$$

The Richardson number criterion is therefore

$$C^{\text{Ri}} = \frac{g\alpha\gamma h^2}{C^{\text{KE}} h^{4/3} \sqrt{g\alpha\gamma} F_b^{1/3}}, \quad (40)$$

$$= \frac{\sqrt{g\alpha\gamma} h^{2/3}}{C^{\text{KE}} F_b^{1/3}}. \quad (41)$$

D Notation

See Table 1 for a brief on the notation used in this document.

References

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