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Mixed Layer Models and Their Application to Water Quality Problems

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Abstract

Four one-dimensional models which have been used to characterize surface mixed layer (ML) processes and the thermal structure are described. Although most any model can be calibrated to mimic surface water temperatures, it does not imply that the corresponding mixing processes are well described. Eddy diffusion or "K" models can exhibit this problem. If a ML model is to be useful for water quality applications, then it must be able to resolve storm events and, therefore, be able to simulate the ML depth, h, and its time rate of change, dh/dt. A general water quality model is derived from mass conservation principles to demonstrate how ML models can be used in a physically meaningful way to address water quality issues.

Introduction

The mixed layer (ML) is the near-isothermal portion of the upper water column which overlies the thermocline and separates the surface from the bottom waters. The bottom waters may too be near-isothermal or it may show relic stratification from earlier episodes of ML deepening and retreat. The thermocline is the transition zone between surface and bottom waters and as such is often thin in its vertical extent and marked by strong gradients in temperature. This stratification in temperature/density has profound effects on circulation and mixing. The success of model simulations of these processes is often limited by how well ML processes have been characterized.

Progress in advancing the understanding of ML dynamics is limited by lack of data suitable for testing and evaluating various theoretical concepts (Müller and Garwood 1988). To fully comprehend ML dynamics, a three-dimensional framework able to directly resolve the influence of Ekman pumping, Langmuir circulation, and diurnal cycling is required. Although much remains to be done, a large amount of useful work has been accomplished with one-dimensional ML models. Some of these accomplishments will be the focus here.

Briefly, to describe the evolution of the thermal structure and its annual cycle requires knowledge of (1) the mechanical energy input into

the water column which tends to destabilize stratification and deepen the ML, and (2) the thermal energy input which tends to stabilize the water column and retard mixing. It is the competition between these two processes, recent and past, which controls the thermal structure. Efforts to numerically simulate these processes began with Munk and Anderson (1948) and have persisted through current times, resulting in several different approaches toward the same objective.

The remainder of this paper will review some representative examples of ML models and illustrate how they may be applied to water quality problems.

The Models

Four basic approaches have been used to describe the thermal structure: (1) turbulence closure models; (2) deterministic solutions; (3) eddy diffusion models; and (4) integrated ML models. All four have evolved from their treatment of the Reynolds terms.

Turbulence closure models solve for the Reynolds terms through higher-order turbulence terms. The resulting triple-correlation products require additional parameterizations and coefficients that must be empirically defined to solve the system of equations. The Mellor and Yamada level 2 1/2 model (Mellor and Yamada 1982) will represent this approach.

Deterministic solutions attempt to directly solve for the Reynolds terms and have been attempted by Deardorff (1970). In general, the fine temporal and spatial resolution requirements do not make this a practical approach and will not be considered here.

Eddy diffusion or "K" models have been popular since Munk and Anderson (1948) first used such a model to describe thermocline formation. The approach has many critics whose concerns range from disbelief that a local relationship exists between mean scalar fields and eddy fluxes (Davis 1983) to a weak theoretical basis and lack of meaningful scale dependence (Batchelor and Townsend 1956; Roberts 1961), and a sentiment that the data base is too weak to formulate the eddy transfer coefficients in terms of a stability parameter (Woods 1977). Nonetheless, because of the continuing popularity of this approach with water quality applications, the McCormick and Scavia (1981) model will be used to represent this class.

Observations on upper ocean structure led Kraus and Turner (1967) to develop a model that exploits the often uniform characteristics of the surface ML. The basic assumption is that there is a "slab" of water that is in equilibrium with the local surface forcing. Model types are further subdivided by their entrainment mechanism. They are turbulent erosion models and dynamic instability models (Cushman-Roisin 1981). The former approach is the Kraus and Turner (1967) model type which scales deepening with an estimate of the energy available for mixing. The latter

approach treats ML deepening to result from shear instabilities in the mean flow and began with Pollard et al. (1973). Two models will be described from this class. The first model (Thompson 1976) is strictly a dynamic instability type model while the second one (Garwood 1977) contains both of these deepening mechanisms.

Therefore, the four models to be examined here are: (1) the Mellor and Yamada (1982) model referred to as "MY21/2"; (2) the McCormick and Scavia (1981) model referred to as "K"; (3) the Garwood (1977) model referred to by the author's initials "RWG"; and (4) the Thompson (1976) model referred to as "RT" in reference to Rhines and Thompson (R.O.R.Y. Thompson, personal communication, 1987).

MY21/2 Model

The version of the MY21/2 model used here employs equations that describe the conservation of heat, momentum, and turbulent kinetic energy (TKE) in the vertical

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial z}(K_m + \nu_m \frac{\partial u}{\partial z}) + fv \tag{1}$$

$$\frac{\partial v}{\partial t} = \frac{\partial}{\partial z}(K_m + \nu_m \frac{\partial v}{\partial z}) - fu \tag{2}$$

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}(K_H + \nu_H \frac{\partial T}{\partial z}) + \frac{1}{\rho_0 C_p}\frac{\partial R}{\partial z} \tag{3}$$

$$\frac{\partial}{\partial t}(\frac{q^2}{2}) = \frac{\partial}{\partial z}[K_q \frac{\partial}{\partial z}(\frac{q^2}{2})] + K_m[(\frac{\partial u}{\partial z})^2 + (\frac{\partial v}{\partial z})^2] + K_H \frac{g}{\rho_0}\frac{\partial \rho}{\partial z} - \frac{q^3}{cl} \tag{4}$$

where

u,v	horizontal velocity components, positive eastward and northward, respectively;
t	time;
z	vertical coordinate, positive upward;

K_m	eddy diffusion coefficient for momentum;
K_H	eddy diffusion coefficient for heat;
$\nu_{m,H}$	background K_m and K_H, respectively;
f	Coriolis parameter;
T	temperature;
ρ_0	reference density;
C_p	specific heat at constant pressure;
R	penetrative component of solar radiation;
$q^2/2$	$(u'u'+v'v'+w'w')/2$ the TKE where the primes denote the fluctuating components of the velocity field;
K_q	eddy diffusion coefficient for TKE;
g	gravitational acceleration;
ρ	density, calculated as a function of T and pressure after Chen and Millero (1986);
l	turbulence length scale; and
c	a constant which modifies l.

The boundary conditions are:

$$(K_m+\nu_m)\frac{\partial u}{\partial z}\Big|_{z=0} = \frac{\tau^x}{\rho_0} \tag{5}$$

$$(K_m+\nu_m)\frac{\partial v}{\partial z}\Big|_{z=0} = \frac{\tau^y}{\rho_0} \tag{6}$$

$$(K_H+\nu_H)\frac{\partial T}{\partial z}\Big|_{z=0} = \frac{Q}{\rho_0 C_p} \tag{7}$$

$$(K_H+\nu_H)\frac{\partial T}{\partial z}\Big|_{z=-H} = 0 \tag{8}$$

where

$\tau^{x,y}$	are the eastward and northward components of the surface wind stress vector τ, respectively, equal to $\rho_a C_d \lvert W \rvert W$;
ρ_a	air density;

H	lake depth;
C_d	stability dependent drag coefficient at 1Om;
W	wind vector; and
Q	surface heat flux.

The eddy coefficients K_m, K_H, and K_q govern the mixing rates within the mixed layer. Ignorance of these processes has led to assuming K_q equal to K_m, and K_m and K_H are calculated by

$$K_m = lqS_m$$
$$K_H = lqS_H \tag{9}$$

where S_m and S_H are stability dependent functions based upon a local Richardson Number.

The last remaining parameter, l, is specified according to the Blackadar boundary layer formula

$$l = [(l_0)^{-1} + (\kappa z)^{-1}]^{-1} \tag{10}$$

where

$$l_0 = (\gamma \int_{-h}^{0} |z| q dz)(\int_{-h}^{0} q dz)^{-1} \tag{11}$$

and κ is Von Karman's constant and equals 0.4. The constant γ is set at 0.2.

K Model

The McCormick and Scavia (1981) eddy diffusion or "K" model can be thought of as a zeroth order turbulence closure model. The basic model is described by

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}(K_H \frac{\partial T}{\partial z}) + \frac{1}{\rho_0 C_p}\frac{\partial R}{\partial z} \qquad -H \le z \le 0 \tag{12}$$

$$K_H = \begin{cases} \dfrac{U_*^3}{\beta g \alpha \kappa^2 z^2 \dfrac{\partial T}{\partial z}} & z \ge -h_T \\ K_H(z = -h_T) & z < -h_T \end{cases} \tag{13}$$

where

- U. friction velocity, equal to $(\tau/\rho_0)^{0.5}$;
- α volumetric expansion coefficient, equal to $-(1/\rho_0)(\partial\rho/\partial T)$;
- h_T depth of minimum thermocline diffusivity; and
- β empirical coefficient.

RWG Model

The RWG model (Garwood 1977) is an integral mixed layer type model that accounts for the two major deepening mechanisms — shear-induced and turbulent erosion. The model is described by

$$0 = m_3 U_*^3 - [\frac{(\Delta u)^2 + (\Delta v)^2}{2}]\frac{\partial h}{\partial t} - m_2(q^2 - 3w'^2)q - \frac{2}{3}(m_1 q^3 + m_5 fhq^2) \tag{14}$$

$$0 = -\alpha g \frac{h}{2}\Delta T \frac{\partial h}{\partial t} + \Phi + m_2(q^2 - 3w'^2)q - \frac{1}{3}(m_1 q + m_5 fh)q^2 \tag{15}$$

$$\Phi = \frac{-\alpha g h}{2\rho_0 C_p}[Q + R(0) + R(-h)] + \frac{\alpha g}{\rho_0 C_p}\int_{-h}^{0} R(z)dz \tag{16}$$

$$\alpha g h \Delta T \frac{\partial h}{\partial t} = m_4 q^2 w' \tag{17}$$

where Δu, $\Delta v = u - u(-h)$, $v - v(-h)$, respectively, and $\Delta T = T - T(-h)$. Following Martin (1985) and McCormick and Meadows (1988) $\partial h/\partial t$ and all terms containing w' are set equal to zero when the ML is shallowing. The constants m_1 and m_5 scale dissipation, m_2 scales the partitioning of TKE between the horizontal and vertical, m_3 scales the surface flux of TKE, and m_4 scales the energy flux at h. Following Garwood (1977), $m_1 = m_2 = m_4 = 1$, and m_3 and m_5 are adjusted to obtain a good fit with data.

RT Model

The RT model (Thompson 1976) is based upon a couple of simple assumptions. If the total shear stress at the ML base is used to accelerate the entrained fluid to the ML velocity, then the momentum equations become

$$\frac{d(hu)}{dt} - fhv = \frac{\tau^x}{\rho_0} \tag{18}$$

$$\frac{d(hv)}{dt} + fhu = \frac{\tau^y}{\rho_0}. \tag{19}$$

Thermal heating is represented by

$$\frac{dT}{dt} = \frac{Q + R(0) - R(-h)}{h \rho_0 C_p} \qquad -h \le z \le 0 \tag{20}$$

$$\frac{\partial T}{\partial t} = \nu_H \frac{\partial^2 T}{\partial z^2} + \frac{1}{\rho_0 C_p} \frac{\partial R}{\partial z} \qquad z < -h \tag{21}$$

In (20), the ML temperature is clearly seen as depth integrated while changes in temperature below the ML (21) are due to a background eddy diffusion, ν_H, and passive heating. These equations essentially represent the Pollard et al. (1973) model. The equations are closed by assuming that the ML flow remains marginally stable. Thompson (1979) reformulated closure in terms of a Froude number, F, and suggested it remain at unity throughout the ML

$$F = \frac{u^2+v^2}{gh\frac{\Delta\rho}{\rho_0}} = 1 \qquad -h <= z \leq 0 \tag{22}$$

The model used here is based on this assumption as well as the further simplification of zero momentum below the ML (Thompson 1976). In practice, this is justified because it is the current shear not magnitude that controls deepening. Without this last assumption, additional parameterizations would be required.

Model Response

Three of the models (K, RT, and RWG) were used in Lake Erie simulations (McCormick and Meadows 1988), and two of the models (MY21/2 and RWG) were used by Martin (1985) in his simulations of North Pacific data. Garwood's original computer code describing Equations 14 to 17 (RWG) was used by both Martin (1985) and McCormick and Meadows (1988) in their simulations which provide a basis for estimating how the MY21/2 model may respond in large lake applications. Both papers describe results from idealized forcing experiments that isolate model response under sustained heating, cooling, and wind forcing conditions. More detailed descriptions of these experiments can be found in those publications.

In general, the models exhibit their greatest similarity under sustained cooling conditions. Here the model physics is dominated by surface generated gravitational instabilities which are removed by adjusting the ML temperature and depth until hydrostatic stability is restored. The exact mixing parameterization employed by the different models is of little consequence in these situations. Under strong heating conditions the models also show strong similarities in their response with each of them forming a shallow mixed layer. The strong positive buoyancy flux into the surface waters retards mixing, and, thus, the different model approaches towards mixing are not highlighted here either.

The greatest difference in model response and the one of greatest consequence to water quality applications occurs under wind-induced

mixing and ML deepening. Three of the models (RWG, RT and MY21/2) are highly correlated to each other in their response to wind deepening of the ML. Although their final ML depths may differ, the response time of the three models to a suddenly imposed wind stress is rapid and similar among these models. The K model, however, showed a limited response to wind forcing. When wind speeds were increased from 1 to 20 m/s the ML depth calculated by the K model increased from 6 to 8 m, whereas the RWG modeled ML deepened from 3 to 57 m under the same conditions (McCormick and Meadows 1988).

The disparity between the K model's response to wind-induced deepening and the response of the other models reflects the different assumptions used to formulate the models and their consequences. For example, the inability of the K model to track storm-induced deepening was clearly demonstrated by McCormick and Meadows (1988) for Lake Erie. During late May 1979, Lake Erie experienced a strong storm which temporarily destroyed lake stratification and mixed the entire water column. In the K model simulation of this storm, stratification and reduced vertical mixing persisted throughout this period while the other models accurately tracked storm related changes in the temperature structure. Although the K model did very well in simulating weekly and longer-term surface water temperatures, it did poorly in describing mixed layer dynamics. During the stratified season, the major mechanism for nutrient replenishment of surface waters occurs via episodic wind-driven events. The failure of the K model to track storm-induced deepening of the surface ML makes it and other models like it poor candidates for water quality applications.

The other three models are suitable for open ocean and large lake applications where rotational effects are important. For applications in smaller water bodies, however, the Dynamic Reservoir Simulation Model (DYRESM) (Imberger et al. 1978) is appropriate. Spigel and Imberger (1980) and Gorham and Boyce (1989) provide useful criteria for determining when basin geometry influences mixed layer dynamics and thus, model choice.

Application to Water Quality Problems

Mixing in water quality models is typically described using a box model where the boundary or boundaries used to segment the water column are fixed and the volumes are constant. Consider the simplest case, a two-box model with a surface concentration of some dissolved tracer at C_1, a bottom concentration at C_2, the total depth being, H, and the mixing length scale being L. The mass flux per unit area between the boxes is $K\Delta C/L$ where K is the dispersion coefficient. There are two problems with this approach. First, the mixing length, L, is arbitrary. The arbitrary boundary introduces dispersion into the problem because vertical homogeneity is imposed where none may exist. This geometry-

induced dispersion leads into the second problem of formulating a meaningful coupling between K and physical measurements. In general, no such link can be made, and, therefore, K must be suitably calibrated for each application.

A better approach to the fixed geometry of the box model is a two compartment mixed layer model. The boundary separating surface from bottom waters is no longer fixed but is time dependent and equal to the ML depth, h, specified from either data or through simulation with an appropriate ML model.

Implementing the mixed layer approach for water quality applications begins by deriving the ordinary differential equations describing the system. The initial mass, M, per unit area of some dissolved tracer is

$$M = C_1 h + C_2(H-h) \tag{23}$$

The dependence of M on h is seen by differentiating (23) with respect to time, which yields after simplification

$$\frac{dM}{dt} = -(C_2-C_1)\frac{dh}{dt} + h\frac{dC_1}{dt} + (H-h)\frac{dC_2}{dt} \tag{24}$$

It should be noted that in (24), dh/dt can be positive or negative. Although dh/dt has been used in ML models to indicate entrainment, which can only be meaningful if positive, it is also used for defining the thickness of the upper and lower regions of the water column. Hence, if mass is to be conserved there can be no constraints on the sign of dh/dt. To avoid possible confusion, separate conservation equations will be written whereby dh/dt will be consistent with its usage in ML models.

For the surface layer

$$\frac{dC_1}{dt} = \frac{SF}{h} + \Lambda_1 \frac{(C_2-C_1)}{h}\frac{dh}{dt} - kC_1 \tag{25}$$

where

SF flux across air/water interface;

k total first-order loss rates; and

$\Lambda_1 \begin{cases} 1 & \text{if } dh/dt > 0 \\ 0 & \text{otherwise.} \end{cases}$

The Λ_1 constraint on dh/dt makes its interpretation consistent with that used in ML models, i.e., influx of C_2 into surface waters can only occur when dh/dt is positive and entrains fluid at C_2.

The bottom layer conservation equation is

$$\frac{dC_2}{dt} = -\Lambda_2 \frac{(C_2 - C_1)}{(H-h)} \frac{d(H-h)}{dt} - \frac{BF}{(H-h)} - kC_2 \qquad (26)$$

where

BF flux across sediment/water interface; and

$\Lambda_2 \begin{cases} 1 & \text{if } d(H-h)/dt > 0 \\ 0 & \text{otherwise.} \end{cases}$

The Λ_2 constraint can be thought of as reverse entrainment. Namely, $\Lambda_2 = 1$ when (H-h) increases, which occurs when the mixed layer retreats due to either a weakening of the wind stress, or when bottom turbulence is sufficiently large for bottom waters to actively entrain the surface layer.

By incorporating a ML model with water quality concerns it establishes a physical basis for defining both the surface layer and exchange with deeper waters. This approach can be easily extended into multiple grids for a more accurate estimate of the vertical mass flux. And finally, additional processes such as a background level of eddy diffusion or particle settling can be easily incorporated without having to alter the basic approach.

Summary and Conclusions

Four one-dimensional models that have been used to calculate the temperature structure of large lakes have been described in a consistent mathematical framework. Most any model can be suitably calibrated to simulate surface water temperatures, yet it is the model's ability to accurately calculate the ML depth, h, and dh/dt that determines its success when applied to water quality problems or in ecological models. Three of the models described here, MY21/2, RT, and RWG, meet these criteria. Finally, a general water quality model was derived from mass conservation principles to demonstrate how ML models can be used in a physically meaningful way to address water quality issues.

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