

# Calculation of Vertical Profiles of Lake-Averaged Temperature and Diffusivity in Lakes Ontario and Washington

MICHAEL J. MCCORMICK AND DONALD SCAVIA

*Great Lakes Environmental Research Laboratory, National Oceanic and Atmospheric Administration, Ann Arbor, Michigan 48104*

By using statistical analysis of temperature observations and model calculations, the common parameterization of vertical eddy diffusivity ( $k$ ) in terms of the gradient Richardson number ( $Ri$ ) is simplified. The simpler formulation accurately reproduces seasonal variations in temperature profiles from Lakes Ontario and Washington. Energy arguments support use of the simplified parameterization and suggest use of a modified  $Ri$  in calculating  $k$ . The new expression for  $k$  resulted in more realistic estimates of thermocline  $k$ . The modeling of free convective mixing in Lake Ontario by heat conservation resulted in excessive temperatures in the hypolimnion during fall overturn.

## INTRODUCTION

Biological and chemical properties of lakes are influenced greatly by physical processes. Boyce [1974] documents the importance of lake physics in understanding the Great Lakes' ecosystems; numerous other examples exist in the literature. For example, influence of Langmuir circulation on primary production [Harris, 1973] and on plankton sedimentation [Titman and Kilham, 1976; Scavia and Bennett, 1980] and of turbulent entrainment on recycling nutrients [Hesslein and Quay, 1973] are recognized as important physical interactions. The complexity of simulating the influence of physical processes on ecosystem dynamics requires appropriate simplifications. In this paper we examine one particular physical phenomenon, vertical transport of heat. Examination and simulation of this process allow us to determine vertical profiles of temperature and to obtain numerical estimates of eddy diffusivities in the epilimnion.

Vertical transport of heat has generally been considered in two ways: (1) a mechanical energy balance approach [e.g., slab models, Kraus and Turner, 1967; Denman, 1973] and (2) a turbulent diffusion approach [e.g., Sundaram and Rehm, 1973; James, 1977]. In general, the former approach models vertical temperature structure by conserving both mechanical and thermal energy in a two-layer fluid. Mixing is instantaneous in the surface layer and is zero in the bottom layer. Changes in mixed-layer depth are controlled by insolation and turbulent energy available for entrainment of bottom water. Although the approach is useful for describing the main, seasonal cycle of thermocline depth and temperature difference, the turbulent diffusion approach is better for investigating smaller-scale vertical exchanges of heat and other materials in the water column.

The turbulent diffusion approach, which we examine herein, parameterizes turbulent mixing in terms of variable eddy diffusivity  $k$ . Vertical and temporal variations of  $k$  govern the temperature profile. Eddy diffusivity is usually parameterized in a manner consistent with its turbulence dependence through some stability parameter (for example, the Richardson or Froude number).

In the present paper we reanalyze a typical formulation of the  $k$  theory approach to thermocline modeling with data from Lake Ontario and Lake Washington. The functional form of  $k$  is reduced to an expression simpler than those used

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by previous investigators, which suggests a modified approach to its estimation. Analysis of this simpler expression identifies the similarities between  $k$  theory and slablike models. We also examine the effects of simulating free convection in turbulent diffusion models.

## MODEL

We begin with the one-dimensional heat diffusion equation

$$\frac{\partial T}{\partial t} = \frac{1}{A} \frac{\partial}{\partial Z} \left( kA \frac{\partial T}{\partial Z} \right) \quad 0 \leq Z \leq H \quad (1)$$

where

- $T$  temperature;
- $A$  cross sectional area as  $f(z)$ ;
- $H$  maximum lake depth;
- $k$  eddy diffusivity;
- $t$  time;
- $z$  depth (positive downward).

Eddy diffusivity is expressed in terms of some stability parameter as

$$k/k_0 = f(s) \quad (2)$$

where  $s$  is a stability parameter and  $k_0$  is the eddy diffusivity under neutral stability. Different formulations of varying complexity for  $k_0$  are used in mixed layer models [Henderson-Sellers, 1976]. Our choice for  $k_0$  was determined by dimensional considerations of the turbulence-energy equation [Kraus, 1972], where under neutrally stable conditions and Reynold's analogy,  $k_0$  can be parameterized in the following fashion:

$$k_0 = cU_* \quad (3)$$

where  $c$  is an appropriate constant proportional to the scale of the primary eddies driving the turbulent cascade and  $U_*$  is the friction velocity which equals  $(C_d W^2 \rho_a / \rho_w)^{1/2}$ , where

- $C_d$  dimensionless wind drag coefficient;
- $\rho_a / \rho_w$  ratio of density of air to the density of water;
- $W$  wind speed.

The stability parameter most commonly used to reflect departures from neutrally stable conditions is the gradient Richardson number ( $Ri$ ). It is usually included in the following way:

$$k = k_0(1 + \sigma Ri)^{-\alpha} \quad (4)$$

where

- $\alpha, q$  constants;  
 $Ri = N^2 / (\partial u / \partial z)^2$ ;  
 $N = [-\alpha g (\partial T / \partial z)]^{1/2}$  (Brunt-Vaisala or buoyancy frequency for fresh water);  
 $\alpha = -(1/\rho)(\partial \rho / \partial T) \sim \alpha_0 (T - 4)$ ;  
 $u$  horizontal water velocity;  
 $\rho$  density of water;  
 $\alpha_0$  volumetric expansion coefficient at an appropriate  $T$ ;  
 $g$  gravitational constant.

Munk and Anderson [1948] and Kent and Pritchard [1959] used values for  $q$  based on different assumptions regarding partitioning of gravitational and mechanical energy in the mixing process. Munk and Anderson [1948] used a value of 1.5, while Kent and Pritchard [1959] use 1.0. Walters *et al.* [1978], while examining heat fluxes using eddy diffusivities in the form of equation (4), suggested use of 1.0 on theoretical grounds. We use this value.

To determine values of the gradient Richardson number, some assumptions need to be made about the velocity shear ( $\partial u / \partial z$ ). Analyses of velocity fluctuation in the mixed layer [Jones and Kenney, 1977] and laboratory experiments [Kato and Phillips, 1969] suggest  $U_*$  as the relevant turbulence velocity scale. However, it is generally recognized that mixed layer deepening is dominated by storm events, and work by Price *et al.* [1978] suggests that the appropriate turbulence velocity scale, under these conditions, is the velocity differential across the bottom of the mixed layer rather than  $U_*$ . Nonetheless we are interested in simulating the thermal structure on a seasonal basis and assume that by time averaging intermittent storm events with stormless conditions we can use  $U_*$  to approximate the turbulence velocity scale for the entire simulation. Time averaging obviously limits model resolution, but it enables us to assume that the velocity shear can be represented by the 'law of the wall':

$$\partial u / \partial z = U_* / Kz \quad (5)$$

where  $K = 0.4$  (Von Karman's constant).

Use of equation (5) theoretically limits model application to the epilimnion because it is strictly valid only for homogenous fluids of shallow enough depth to be unaffected by rotation. We assume that in lakes with shallow thermoclines (relative to oceanic conditions), buoyancy forces rather than rotational effects will dominate in limiting vertical transfer of momentum. Therefore we ignore rotational effects in calculating eddy diffusivity.

The wind drag coefficient ( $C_d$ ) used in the calculation of  $U_*$ , both in equation (5) and for approximation of  $k_0$ , is applied herein in two different ways: (1) it is held constant, and (2) it is allowed to vary as a function of wind speed and atmospheric stability. Below we give results of testing both approaches.

We combine the results for approximation of the eddy diffusion:

$$k = \frac{cU_*}{[1 - \sigma Kz^2 \alpha (\partial T / \partial z) / U_*^2]} \quad (6)$$

In order to obtain a best fit to observations (in a least squares sense) we used a nonlinear regression algorithm to estimate the two constants ( $\sigma, c$ ) in equation (6). No unique set of optimal parameters could be found. Analysis of the response surface of the objective function (sum of squares of deviations of

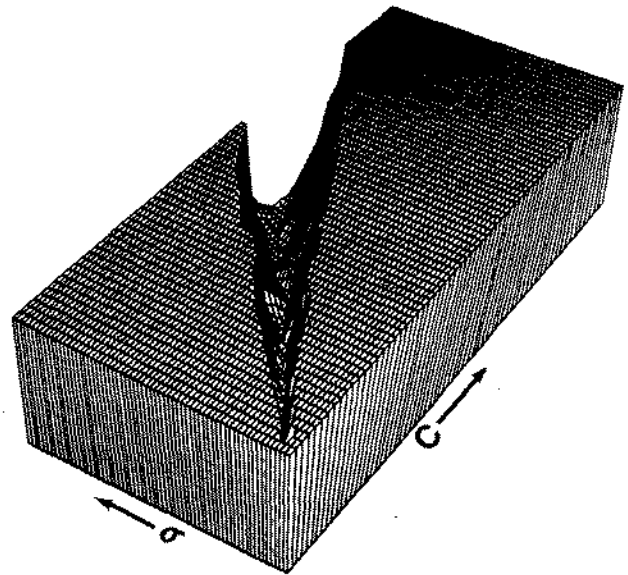


Fig. 1. Planar section of the response surface of the sum of squares statistic as a function of  $\sigma$  and  $c$ . The valleylike feature corresponds to the optimal values of  $\sigma$  and  $c$  for minimizing the sum of squares. Any pair of values of  $\sigma$  and  $c$  lying in the trough represents a local minimum. The continuous and linear nature of the valley shows that  $\sigma$  and  $c$  are highly correlated ( $r = 0.97$ ).

model from data) versus the parameters  $\sigma$  and  $c$  (Figure 1) indicated that the objective function could be minimized apparently with a very large number of parameter combinations. In minimizing the sum of squares,  $\sigma$  and  $c$  are highly correlated ( $r = 0.97$ ), which indicates that the ratio  $\sigma/c$  is constant.

When data from additional numerical experiments were considered, the ratio remained constant for values of  $c$  ranging from slightly greater than zero to arbitrarily large. This allowed us to reformulate the expression for eddy diffusivity in a simpler way. If equation (6) is rearranged such that

$$k = \frac{U_*}{(1/c) + (\sigma/c) Ri}$$

and  $c$  becomes very large, then

$$k = U_* / \beta Ri \quad (7)$$

where  $\beta = \sigma/c$  is a constant. This formulation is similar to that proposed by Kullenberg *et al.* [1973] based on experimental dye studies in Lake Ontario.

#### Limits to $k$

As the water column begins to stratify, parameterization of  $k$  as given by equations (6) or (7) cannot be used explicitly in the hypolimnion since it would violate the assumptions used in specifying shear stress. Ignorance of the shear stress in and below the thermocline and of how it is coupled to surface stress requires either of two approaches. One approach is to use different  $k$  parameterizations for each layer. For example, Walters *et al.* [1978], in modeling the thermal structure of Lake Washington, limited the Kent and Pritchard [1959] formulation [equation (4)] to the epilimnion, used the Jassby and Powell [1975] formulation ( $k \propto (N^2)^{-0.4}$ ) in the upper hypolimnion, and used a constant diffusivity, equal to 10 times the thermocline minimum or the surface value (whichever is smaller), in the remainder of the hypolimnion.

The second approach, which we use here, is simpler and assumes  $k$  to be constant in the hypolimnion. Selection of the constant  $k$  has ranged from choosing molecular diffusion values [Dake and Harleman, 1969] to choosing the thermocline minimum of the calculated eddy diffusivity [Sundaram and Rehm, 1973]. Following this latter approach we set all diffusion coefficients below a critical depth  $h$  equal to the thermocline minimum as follows:

$$\frac{\partial T}{\partial t} = \frac{1}{A} \frac{\partial}{\partial z} \left( k' A \frac{\partial T}{\partial z} \right) \quad (8)$$

where

$$k' = k(Z) \quad Z \leq h$$

$$k' = k(h) \quad Z > h$$

and  $h$  is the depth of minimum thermocline eddy diffusivity. Equation (8), with  $k$  defined by equation (7), is solved with an explicit, finite, centered-difference scheme subject to the following boundary conditions:

$$T(0, t) = T_s(t) \quad t > 0$$

$$\partial T / \partial t (H, t) = 0$$

$$T(Z, 0) = T_i(Z)$$

$$U_* = (c_d W^2 \rho_a / \rho_w)^{1/2}$$

where  $W$  is the time dependent wind speed at the surface,  $T_s(t)$  is the specified surface temperature,  $H$  is the maximum lake depth, and  $T_i(Z)$  is the initial temperature profile.

#### Free Convection

Response time of this finite difference approximation for equation (8) to gradually varying heat fluxes is not excessive, provided that large-scale hydrostatic instabilities do not occur. Sundaram and Rehm [1973] handled these instabilities by setting all diffusion coefficients from the surface downward equal to the first subsurface peak in  $k$ , provided it exceeded the surface value. This method works satisfactorily for diurnal convection due to nocturnal cooling of surface layers, but is inadequate for modeling larger-scale convection such as that occurring during fall overturn. We simulate full penetrative convection by using a heat balance approach. Whenever surface cooling occurs, resulting in hydrostatic instabilities, the 'excess' heat contained in the unstable region is mixed with cooler water below until a stable density gradient is restored. With sustained surface cooling, as in the fall, temperature profiles resulting from the heat balance calculation alone are indicative of conservation of potential energy in the mixed layer because the thermocline has been weakened and deepened.

## RESULTS

### Lake Ontario

For simulation of Lake Ontario, lakewide averaged daily surface temperatures [Pickett, 1975] were used as the surface boundary condition, zero heat flux was used at the bottom boundary, and a constant 4°C temperature was used as the initial condition (April 8, 1972). Variation of area with depth was approximated by

$$A(z) = 1.11 \times 10^{-5} Z^2 - 6.66 \times 10^{-3} Z + 1 \quad 0 \leq Z \leq 180$$

where  $Z$  is depth in meters and  $A$  is dimensionless. Wind

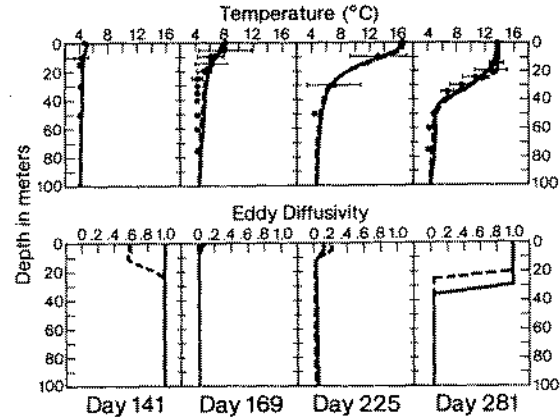


Fig. 2. Temperature and dimensionless eddy diffusion profiles for Lake Ontario. The solid lines are obtained with a constant drag coefficient, and the dotted lines are obtained with a variable drag coefficient. Observed values are represented by dots  $\pm 1$  standard deviation. The dimensionless eddy diffusion coefficients  $k$  are determined by dividing  $k$  by the numerical stability criterion (i.e.,  $\max k \leq (\Delta z)^2 / \Delta t$ ).

stress values were calculated from wind speed data measured over Lake Ontario [Pickett, 1975]. The model was numerically integrated with a time step of 4 hs and a vertical resolution of 5 m.

Using equation (7) for  $k$ , a constant wind drag coefficient ( $C_d = 0.0015$ ) and  $\beta = 3.5 \times 10^{-4}$ , we obtained temperature and diffusivity profiles (Figure 2). The observations are lake-wide averaged, three-day means  $\pm 1$  standard deviation. The examples of simulated temperature profiles in Figure 2 are representative of the full data set and agree well with observations (rms = 0.84). The diffusivity profiles are what one might expect for a stably stratified system except that the simulated diffusivities do not increase in the hypolimnia due to the limitations imposed by equation (8). The annual cycle of development, growth, and destruction of the thermocline from early spring through late fall is well described. In general, the largest deviations from observations occurred in the lower thermocline region with typical differences of 1–2°C between modeled and observed temperatures. Calculated profiles are well within the variability in the data demonstrating the adequacy of equation (7) for estimating  $k$ .

We examined the effect of a variable wind drag coefficient  $C_d(s)$  to see if an even better fit could be achieved between modeled and observed temperatures for Lake Ontario. We used 89 different values of  $C_d$ , calculated from three-day averages of wind speed and air-sea temperature difference from April through November by a method described by Schwab [1978]. A single drag coefficient ( $1.5 \times 10^{-3}$ ) was used for December through March because of the paucity of data during this period. The variable drag coefficient was lowest in spring and reached its maximum in fall, inversely following the general pattern of atmospheric stability. The variable drag coefficient produced only minor improvements in simulated temperature profiles for Lake Ontario over use of the constant drag coefficient for a coarse grid ( $\Delta Z = 5$  m) and produced essentially no improvement for the case of a finer ( $\Delta Z = 2.5$  m) grid. Eddy diffusivities did respond to differences in the drag coefficient; however, differences in diffusion coefficients calculated via the two approaches were not persistent enough in time to be manifest in the temperature profiles. This suggests a

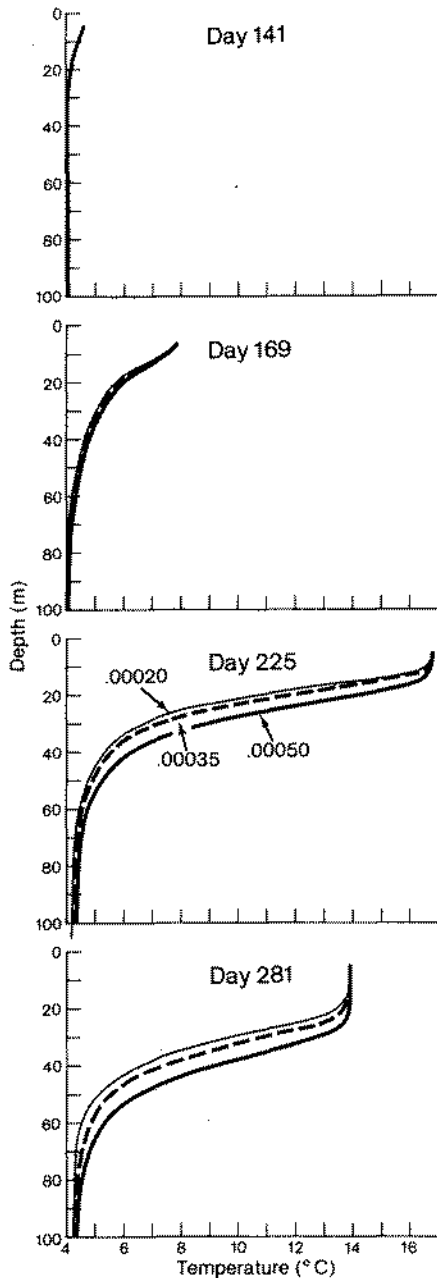


Fig. 3. Sensitivity of simulated temperature profiles for Lake Ontario to  $\beta$ . The profiles correspond to  $\beta$  values of 0.00020, 0.00035, and 0.00050. The optimum value for  $\beta$  is 0.00035.

certain latitude in the selection of  $\beta$ . Two additional simulations were performed for Lake Ontario using values for  $\beta$  that were approximately  $\pm 50\%$  of the optimum value. The resulting temperature profiles show the thermocline depth to be inversely proportional to the magnitude of  $\beta$  (Figure 3).

Additional simulations were performed for Lake Ontario with the depth integrated mean temperature  $\bar{T}(Z, t)$  in place of the local temperature  $T$  in the  $\alpha_0(T - 4)$  term. (The motivation for doing this is explained later.) The simulated temperature profiles were generally improved (rms = 0.73) over prior attempts, and lower estimates of eddy diffusivities in the thermocline were obtained.

During periods of sustained surface cooling, when mixing is

dominated by free convection, the resulting temperature profiles for Lake Ontario showed good agreement with observations in the upper layers but excessive heating of the lower hypolimnion. Temperature excursions in the lower hypolimnion were greatest during fall overturn, when simulation temperatures rose from their nearly constant  $4^\circ\text{C}$  to almost  $4.5^\circ\text{C}$  in contrast to the constant actual temperatures of  $4^\circ\text{C}$ . This implies that fully penetrative convection (i.e., heat conservation) is not predominant during thermocline erosion but rather nonpenetrative or slightly penetrative convection is responsible. This result is consistent with Gill and Turner's [1976] conclusions and suggests that the thermocline acts as a partial barrier restricting the vertical extent of both forced and free convective mixing.

#### Lake Washington

To further test the adequacy of the simpler expression for  $k$  and the dependency of  $\beta$  on different driving conditions, we applied equation (1) (i.e., no hypolimnetic limitation for  $k$ ), with  $k$  defined by equation (7), to the much smaller Lake Washington. Wind speed and morphometry for Lake Washington were obtained from Walters [1977] and temperatures were obtained from J. T. Lehman (personal communication). The period of calculation was from February 1963 to January 1964, and a time step of 4 h, a vertical grid scale of 2.5 m, and  $C_d$  of 0.0015 were used. The initial temperature profile was uniform at  $7.2^\circ\text{C}$ . Results (Figure 4) suggest that the simpler expression for  $k$  (using  $\beta = 1.6 \times 10^{-3}$ ) is also applicable for Lake Washington. One interesting observation is that it was not necessary to limit flux across the thermocline (equation (8)) for Lake Washington as was needed for Lake Ontario. Although this violates model assumptions when the lake is stratified, it resulted in closer agreement with observed hypolimnion temperatures. Because this is contrary to the expected poor results, it suggests the presence of mixing mechanisms other than surface-induced mixing in the hypolimnion. In shallow lakes with shallow thermoclines, like Lake Washington, mixing resulting from bottom friction can be an important mechanism for transporting heat throughout depth [Simpson and Hunter, 1974; James, 1977]. Large values of  $k$  in Lake Washington's hypolimnion may be correct, but since they were obtained in an artificial fashion a more physically inclusive model is required to resolve the specific process.

#### DISCUSSION

Insight into this  $k$  theory approach can be obtained by examining equation (7) in a two layer framework. Ignoring areal effects and integrating equation (1) from the surface to depth  $h$ , corresponding to the depth of the thermocline minimum of the eddy diffusivity,  $k_h$ , and substituting equation (7) for  $k$  we obtain:

$$\int_0^h \frac{\partial T}{\partial t}(z, t) dz = G - \frac{U_*^3}{\beta' g \alpha_0 (T(h, t) - 4) h^2} \quad (9)$$

where  $G = -k \partial T / \partial z|_{z=0}$  (the flux from the surface), and  $\beta' = K^2 \beta$ . By the general Leibnitz Rule, equation (9) can be expressed as

$$\frac{d}{dt} \int_0^h T(z, t) dz = G - \frac{U_*^3}{\beta' g \alpha_0 (T(h, t) - 4) h^2} + T(h, t) \frac{dh}{dt} \quad (10)$$

where  $dh/dt$  represents the entrainment velocity at the

thermocline. Equation (10) can be rewritten as

$$h \frac{d\bar{T}}{dt} = G - D + T(h, t) \frac{dh}{dt} \quad (11)$$

where  $d\bar{T}/dt = (1/h)(d/dt) \int_0^h T(z, t) dz$  and

$$D = \frac{U_*^3}{\beta' g \alpha_0 (T(h, t) - 4) h^2}$$

The left hand side of equation (11) is the time rate of change of the heat content of the mixed layer, and the terms on the right hand side are related to mechanical stirring, energy dissipation, and entrainment, respectively.

Equation (11) is fundamentally identical to the slab models of Kraus and Turner [1967] and Denman [1973] with internal heating ignored. The mixed-layer depth  $h$  for equation (11) is determined by the depth of  $k_*$  rather than by the equilibrium depth of the mechanical-thermal energy equations as for slab models. Nonetheless there exist strong similarities between these slab models and this formulation of  $k$  theory. Agreement between approaches and the reliance on simple physical arguments for development of the slab models provide support for the validity of this  $k$  theory formulation and a different context to examine  $k$  dependencies.

For example, over any time step,

$$\frac{U_*^3 \Delta t}{\beta' g \alpha_0 (T(h, t) - 4) h^2} \quad (D \text{ term})$$

is proportional to the rate of production of mechanical energy divided by the buoyancy of the layer. When  $dh/dt$  is negligible compared to  $G - D$ , then  $G - D$  can be interpreted as representing the energy available for increasing the potential energy of the mixed layer. In order for  $D$  to be consistent with its use in these slab models the temperature used to calculate the layer's buoyancy should be the average epilimnion temperature  $\bar{T}(h, t)$  rather than the local temperature  $T(h, t)$ . This increases  $G - D$ , making more energy available to heat up the mixed layer and therefore less heat fluxed into the hypolimnion. For the  $k$  theory this suggests use of a modified gradient Richardson number to calculate  $k$ , where  $\bar{T}(Z, t)$  replaces the local temperature  $T(Z, t)$ . This effectively accounts for energy loss due to buoyancy forces which mechanical energy input must work against, resulting in lower estimates of  $k$ . Improved simulations of temperature data from Lake Ontario were accomplished by using this approach and resulted in lowered estimates of the seasonally averaged  $k_*$  by approximately one third. This implies that the gradient Richardson number overestimates  $k_*$  and thus overestimates mixing across the thermocline.

#### SUMMARY AND CONCLUSIONS

During sustained episodes of free convective mixing, use of a heat conservation approach to eliminate gravitational instabilities resulted in excessive temperature excursions in the hypolimnion of Lake Ontario. Better agreement with observations should be obtained by using a nonpenetrative or slightly penetrative convection model rather than by using one which conserves heat.

A common parameterization of the eddy diffusivity based on Keni and Pritchard's [1959] formulation was reduced to a simpler expression by statistical comparison of simulated and observed temperatures. The credibility of this expression was supported by identifying its relationship to slablike models.

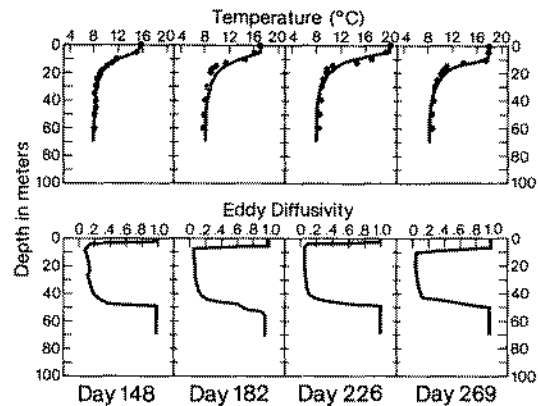


Fig. 4. Temperature and dimensionless eddy diffusion profiles for Lake Washington. The initial temperature profile on day 35 was uniform at 7.2°C (same as Figure 2).

This comparison also provided a mechanism to suggest that improvements in estimating eddy diffusivities may be made by using a 'modified' gradient Richardson number.

For simulation of existing data this  $k$  formulation is preferable to slab models since it has fewer data requirements when the surface temperature is prescribed. Furthermore, by knowing the relationship between  $k$  theory and slablike models and by investigating other lakes it may be possible to establish the functional dependence of  $\beta$ , and thus enable this  $k$  formulation to be used as a predictive tool.

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