One-dimensional, integral energy model

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Model description

A one-dimensional, integral energy model was developed to simulate the temperature, heat flux and stratification dynamics of Lake Mendota as driver for the water quality dynamics. The algorithms are based on the MINLAKE (Ford and Stefan 1980, Riley and Stefan 1988, Herb and Stefan 2004) and the MyLake (Saloranta and Andersen 2007) models. As the focus is on simulating lake thermal dynamics, the model neglects any inflows and outflows, mass losses due to evaporation and water level changes:

$$\frac{\partial h}{\partial t} = 0 \tag{1}$$

where h is the water level and t the time. Heat transport is implemented through the one-dimensional temperature diffusion equation:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial T}{\partial z}\right) + \frac{H(z)}{\rho_w c_p} + \frac{H_{geo}(z)}{\rho_w c_p} \tag{2}$$

where K_z is the vertical turbulent diffusion coefficient, H is internal heat generation due to incoming solar radiation, ρ_w is water density, c_p is specific heat content of water, and H_{geo} is internal geothermal heat generation. Internal heat generation is implemented as:

$$H(z) = (1-\alpha)(1-\beta)I_s \exp(-K_d z) \tag{3}$$

where α is the fraction of reflected incident solar radiation, β is the fraction of infrared radiation, I_s is total incident short-wave radiation, and K_d is a light attenuation coefficient.

For the upper, surface boundary condition we assume a Neumann type for the temperature diffusion equation:

$$\rho_w c_p \left(K_z \frac{\partial T}{\partial z}\right) = H_{net} \tag{4}$$

where H_{net} is the net heat flux exchange between atmosphere and water column:

$$H_{net} = H_{sw} + H_{lw} + H_{lwr} + H_v + H_c \tag{5}$$

where H_{sw} is the incoming solar incident radiation, $H_{sw} = (1-\alpha)I_s$, H_{lw} is the incoming long-wave radiation, H_{lwr} is emitted radiation from the water column, H_v is the latent heat flux, and H_c is the sensible heat flux. Implementations to estimate the respective heat fluxes were taken from Livingstone and Imboden (1989), Goudsmit et al. (2002), and Lerman et al. (1995).

The lower, sediment boundary condition was prescribed as:

$$\left(K_z \frac{\partial T}{\partial z}\right) = 0 \tag{6}$$

The one-dimensional temperature diffusion equation had two options for discretization, either using an explicit FTCS scheme or the implicit Crank-Nicholson scheme, the latter being second-order in both space and time allowing the modeling time step to be dynamic without stability issues (see "Numerical scheme").

The model algorithm is modularized into five components: (a) heat generation from boundary conditions, (b) vertical diffusion, (c) mixed layer depth, (d) convective overturn, and (e) ice formation.

(a) Heat generation from boundary conditions

In the first step the heat fluxes H, H_{geo} and H_{net} are applied over the vertical water column.

(b) Vertical diffusion

In the second step, vertical turbulent diffusion between adjacent grid cells is calculated. Here, we applied a centered difference approximation for temperature at the next time step. The vertical turbulent diffusion coefficient K_z is calculated based on the empirical equations by Hondzo and Stefan (1993) as a function of the buoyancy frequency:

$$K_z = a_k (N^2)^{-0.43} \tag{7}$$

where a_k is an empirical factor accounting for the surface area of the lake A_s:

$$a_k = 0.00706 (A_s)^{0.56} \tag{8}$$

and N^2 is the squared buoyancy frequency:

$$N^2 = \frac{g}{\rho_w} \frac{\partial \rho_w}{\partial z} \tag{9}$$

and values of N^2 less than 7.0 10^{-5} s^{-2} were set to 7.0 10^{-5} s^{-2}.

(c) Mixed layer depth

In the third step, we quantify the depth where the amount of external kinetic energy by wind shear stress equals the internal potential energy of the water column. Up to this depth, adjacent layers are subsequently mixed to account for a wind shear stress acting over the vertical water column. Here, the kinetic energy *KE* is described as:

$$KE = \tau u^* \Delta t \tag{10}$$

where τ is the surface turbulent shear stress, and u^* is the surface shear velocity, which was calculated from wind velocity as:

$$u^* = \sqrt{\frac{C_{10}\rho_a}{\rho_w}}U_2 \quad (11)$$

where C_{10} is the wind stress coefficient dependent on the measured wind speed U_2 at 2 m height above the water surface, and ρ_a is the density of air, respectively (Herb and Stefan, 2005). The potential energy of the water column for each layer over the depth is calculated as:

$$PE_z = gz_z(z_{z+1} - z_{cv})\Delta\rho \quad (12)$$

where g is gravitational acceleration, z_{cv} is the center of volume depth, and $\Delta\rho$ is a density change from the current layer to the next layer below. The mixed layer depth is calculated by incrementally increasing the comparison between the total kinetic energy *KE* and the internal potential energy *PE* as:

$$z_{ml} \rightarrow PE_{z+1} > KE \quad (13)$$

(d) Convective overturn

In the fourth step, any density instabilities over the vertical water column are mixed with a first stable layer below an unstable layer. Here, we applied an area weighed mean of temperature between two layers.

(e) Ice formation

In the fifth step, the ice algorithm from MyLake (Saloranta and Andersen 2007) was applied to the model. Whenever water temperatures were equal or below freezing point water temperatures of 0 °C, ice formation got triggered. All layers with lower water temperatures were set to freezing point temperature, and the heat deficit from atmospheric heat exchange was converted into latent heat of ice formation. When air temperatures were over freezing point temperatures, ice growth ceased, and ice melting got initiated. Here, total energy of ice melting was taken from the total heat flux H_{net}. Once the ice layer has disappeared, the default model routine continued. As the ice module was implemented to prevent the simulation of physically unrealistic water temperatures during the winter-spring seasons, we only focused on a one-layer implementation, i.e., only the formation and melting of ice.

Numerical scheme

An explicit and an implicit scheme were implemented to solve the one-dimensional, temperature transport equation (eq. 1).

Explicit FCTS scheme

The explicit finite different method, Forward Time Centered Space (FTCS), is a first-order method in time, in which Taylor's theorem is applied to approximate the solution of the second-order differential $\frac{\partial^2 T}{\partial z^2}$:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + O(a^4) \quad (14)$$

A central-difference scheme in space *i* (sum of forward and backwards differencing) is then applied for the temperature *T*:

$$T_{i+1} = T_i + \frac{\partial T}{\partial z}\frac{\Delta z}{1!} + \frac{\partial^2 T}{\partial z^2}\frac{\Delta z^2}{2!} + \frac{\partial^3 T}{\partial z^3}\frac{\Delta z^3}{3!} + O(z^4) \tag{15}$$

$$T_{i-1} = T_i - \frac{\partial T}{\partial z}\frac{\Delta z}{1!} + \frac{\partial^2 T}{\partial z^2}\frac{\Delta z^2}{2!} - \frac{\partial^3 T}{\partial z^3}\frac{\Delta z^3}{3!} + O(z^4)$$

$$T_{i+1} - T_{i-1} = 2T_i + \frac{\partial^2 T}{\partial z^2}\frac{\Delta z^2}{2!} + O(z^4)$$

$$\frac{\partial^2 T}{\partial z^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta z^2} + O(z^4)$$

For time *n*, we apply a forward-differencing scheme:

$$\frac{\partial T}{\partial t} = \frac{T_i^{n+1} - T_i^n}{\Delta t} = K_z \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta z^2} \tag{16}$$

Finally, we get an explicit solution as:

$$T_i^{n+1} = T_i^n + K_z \frac{\Delta t}{\Delta z^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n) \tag{17}$$

Implicit Crank-Nicholson scheme

The implicit Crank-Nicholson scheme, which is second-order derivative in space and time, was applied to solve the one-dimensional, temperature transport equation (eq. 2). Here, we average the response in space between the current and the next time step:

$$T_i^{n+1} = T_i^n + K_z \frac{\Delta t}{\Delta z^2}\left[\frac{(T_{i+1}^n - 2T_i^n + T_{i-1}^n) - (T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1})}{2}\right] \tag{18}$$

We let $\alpha = K_z \frac{\Delta t}{\Delta z^2}$ to get:

$$-\alpha T_{i+1}^{n+1} + 2(1+\alpha)T_i^{n+1} - \alpha T_{i-1}^{n+1} = \alpha T_{i+1}^n + 2(1-\alpha)T_i^n + \alpha T_{i-1}^n \tag{19}$$

which is a tridiagonal matrix with nonzero elements on the main diagonal, the first diagonal below, and the first diagonal above the main diagonal only. We can restructure the system as (here, idealized as a 4x4 matrix, assuming that we only have four vertical grid cells):

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ -\alpha & 2(1+\alpha) & -\alpha & 0 \\ 0 & -\alpha & 2(1+\alpha) & -\alpha \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \end{pmatrix} = \begin{pmatrix} T_1^n \\ \alpha T_1^n + 2(1-\alpha)T_2^n + \alpha T_3^n \\ \alpha T_2^n + 2(1-\alpha)T_3^n + \alpha T_4^n \\ T_4^n \end{pmatrix} \tag{20}$$

which can be solved as a linear system using Gaussian elimination through tridiagonal matrix algorithm. Note that we assume no diffusion at the surface and bottom boundaries of the system.

Model verification

The described one-dimensional, integral energy model for temperature and stratification dynamics was applied to Lake Mendota to verify that it can be used as a model driver for a water quality model in a two-way feedback interaction. Observed water temperature data were obtained from the North Temperate Lakes US Long-Term Ecological Research Network (NTL-LTER, https://lter.limnology.wisc.edu/). As the water quality model itself is a vertical, two-layered model that assumes idealized completely-mixed layers in the epilimnion and hypolimnion of a lake, we area weighed the vertical temperature output data. Simulated water temperatures were area weighed either from the surface to the depth of the center of buoyancy (representing the idealized thermocline depth), or from the depth of the center of buoyancy to the sediment boundary. We ran the model from 2009-01-01 to 2009-12-31 with a time step of 3600 s and a space discretization of 1 m.

The model replicates sufficiently the dimictic stratification dynamics of Lake Mendota (Fig. 1) and can replicate the general thermal dynamics of an idealized epilimnion and hypolimnion (Fig. 2). A caveat is that our model has a bias to underestimate heat transport and mixing during spring and fall overturn (Fig. 2) resulting in a discrepancy in water temperature dynamics. Nonetheless, as the main focus for the water quality studies is on the time-dependent entrainment dynamics over the thermocline, our one-dimensional, integral energy model – although a simplified numerical scheme – can sufficiently replicate the stratification dynamics (Fig. 1) as well as the thermocline depths (Fig. 3) of Lake Mendota.

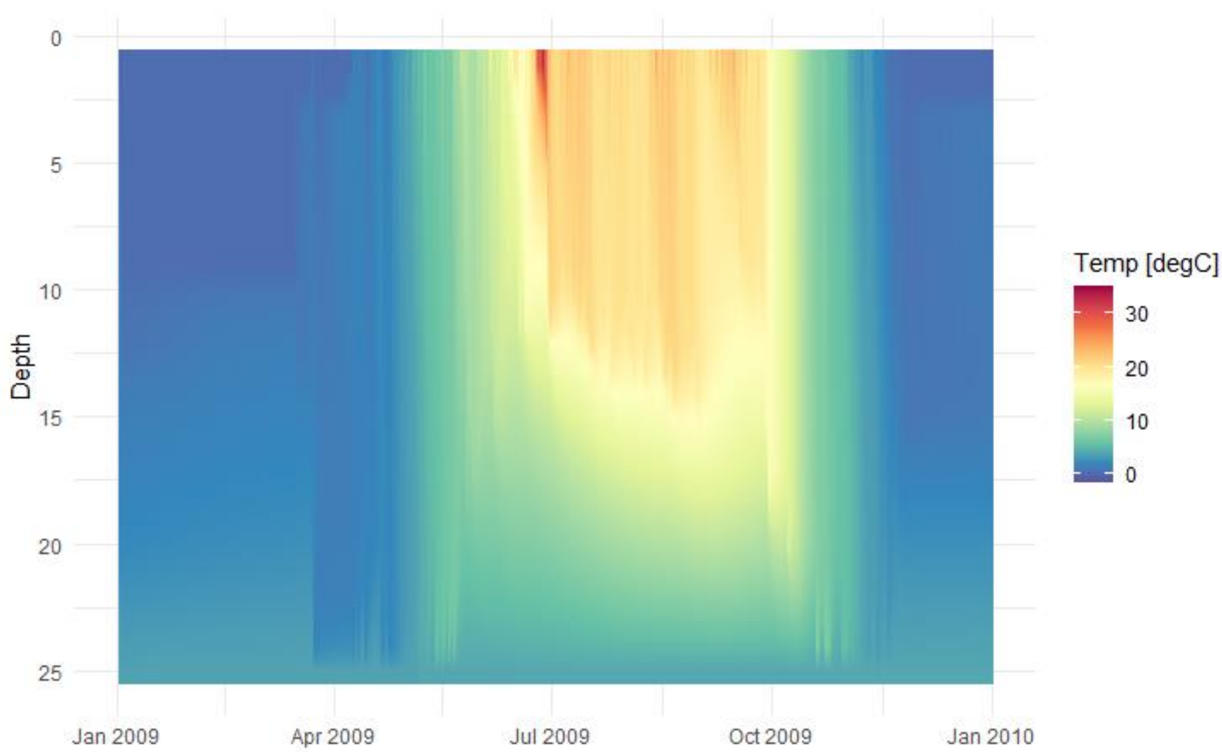

Figure 1 Heat map of simulated water temperatures for Lake Mendota.

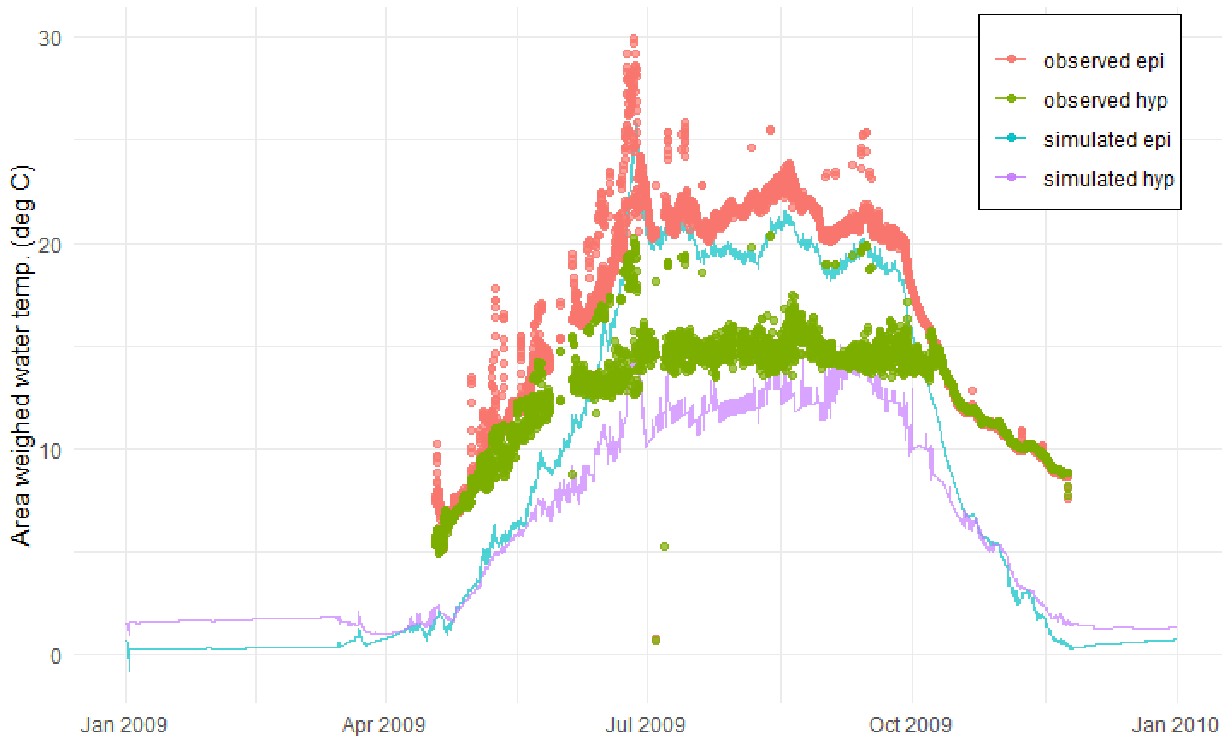

Figure 2 Comparison of area weighed observed water temperature to area weighed simulated water temperature.

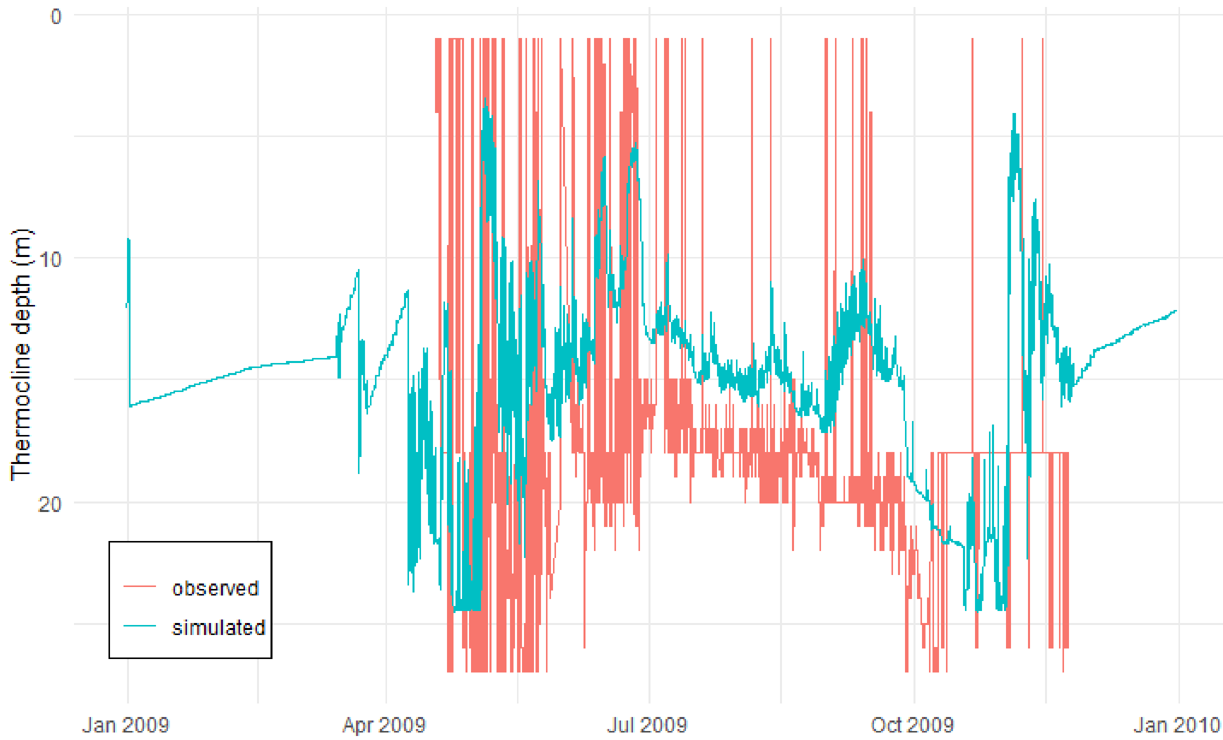

Figure 3 Comparison of observed thermocline depth to simulated thermocline depth. Note that the thermocline depth was calculated as the center of buoyancy depth of the water column.

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