JOURNAL OF LIMNOLOGY

DOI: 10.4081/jlimnol.2016.1447

SUPPLEMENTARY MATERIAL

Contribution of extreme meteorological forcing to vertical mixing in a small, shallow subtropical lake

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Supplementary I

FUNDAMENTAL EQUATIONS

The wind shear stress and net heat flux were calculated from theoretical and empirical equations using the observed data. Using the 2 m height wind speed (W_2) measured in the field, the wind shear stress (in N m^{-2}) at the surface is given by:

$$\tau = \rho_a u_*^2 , \qquad (1)$$

where ρ_a is the air density (kg m^{-3}) and u_* is the surface friction velocity under the assumption of a neutral MET condition (*e.g.* Yu *et al.*, 1983). It is given by the logarithmic neutral profile formula at a height of 2 m:

$$u_* = \frac{kW_2}{\ln(2/z_0)} ,$$

with the von Karman constant k = 0.4 and the roughness height of the water surface ($z_0 \sim 1 \times 10^{-3}$ m reported by Arya 2001). When the net heat flux is computed, it is necessary to use the wind speed at 10 m height (W_{10}). With a logarithmic formula, the wind speed is given by:

$$W_{10} = \frac{\ln(10/z_0)}{\ln(2/z_0)} W_2 .$$

The net heat flux (W m^{-2}) on the water surface (Knauss, 1996), including solar radiation, is given by

$$H_{net} = H_{sw}(1-\alpha_{sw}) + H_{lw} - H_e \pm H_c , \qquad (2)$$

where H_{sw}, H_{lw}, H_e, and H_c (W m^{-2}) are the shortwave radiation, net longwave radiation, latent heat flux, and sensible heat flux, respectively, and α_{sw} is the albedo of shortwave radiations, ranging form 0.06 to 0.10, depending on the zenith angle and water surface conditions, reported by Serreze and Barry (2005). The empirical and theoretical equations used to determine these terms are described in the following paragraphs.

H_{lw} is the Stefan-Boltzmann equation modified by several environmental factors:

$$H_{iw} = \lambda\left[\left(1-\alpha_{lwa}\right)9.37\times10^{-6}T_a^6\left(1.0+0.17C^2\right)-\varepsilon_w T_s^4\right],$$

where ε_w is the emissivity of the water body (0.97), λ is the Stefan-Boltzmann constant (5.67 × 10^{-8} W °K^{-4} m^{-2}), T_a is the air temperature (K), T_s is the surface water temperature (K), α_{lwa} is the albedo of incoming longwave radiation (equal to 0.03 as determined by Henderson-Sellers, 1986), and C is the cloud cover fraction (0 to 1). With the empirical approximation (Fischer, 1979; Colomer *et al*., 1996), H_e is given by

$$H_e = c_e\rho_a L_E W_{10m}(e_s - e_a)/p_a,$$

where C_e is a dimensionless coefficient (1.3 × 10^{-3}) (Pond *et al*., 1971; Hicks, 1972; Kondo, 1975), L_E is the heat of vaporisation (2.45 × 10^6 J kg^{-1}), e_a is the air vapour pressure (hPa) at T_a, e_s is the vapour pressure (hPa) at T_s, and p_a is the air pressure (hPa). H_c is the empirical relationship (Fischer, 1979) given by

$$H_c = c_c c_{pa}\rho_a W_{10m}(T_a - T_s),$$

where c_c is a dimensionless coefficient (1.3 × 10^{-3}) (Pond *et al*., 1971; Hicks, 1972; Kondo, 1975) and c_{pa} is the specific heat capacity of air (1006 J kg^{-1} °C^{-1}).

The Schmidt stability (S_t [J m^{-2}]) defined in Idso (1973) was used as the indicator in our study, and it is given as

$$S_t = \frac{g}{A_0}\int_0^{z_m}(z - z_E)A(z)[\bar{\rho} - \rho(z)]dz, \quad (3)$$

where $\bar{\rho}$ is the mean density (kg m^{-3}) over the lake, z_E is the height (m) at $\bar{\rho}$ from the bottom, z is the height (m) from the lake bottom, z_m is the maximum height (m), $\rho(z)$ is the density (kg m^{-3}) at z, computed by the UNESCO equation of state with water temperature and zero salinity (UNESCO, 1981), A_0 is the surface area of the lake (m^2), and $A(z)$ is the area at z (m^2). The height of the thermocline (z_t) from the water surface is defined by:

$$z_t = z_m - z_E.$$

For surface layer mixing, defined in this study as the mixing that occurs between the lake surface and the upper thermocline, the penetrative convection velocity, w_* (m s^{-1}) and water friction velocity, u_{*w} (m s^{-1}), were used to understand which friction velocity was dominant. The former is related to the buoyancy force and indicates mixing by cooling (Deardoff, 1970). The latter is yielded from wind inputs and indicates mixing by wind-induced turbulence. These velocities are described respectively by:

$$w_* = \left(-\alpha g z_t H_{net} / \rho_0 c_p\right)^{1/3}, \tag{4}$$

where ρ_0 is the water density (kg m^{-3}), c_p is the specific heat capacity of water (4186 J kg^{-1} °C^{-1}), g is the acceleration of gravity (m s^{-2}), α is the coefficient of thermal expansion (°C^{-1}), and

$$u_{*w} = (\tau / \rho_0)^{1/2}. \tag{5}$$

The ratio of the friction velocity to the convection (u_{*w}/w_*) indicates whether contributions from w_* or from u_{*w} are the dominant source of turbulent energy to the SML (Read *et al.* 2012). The threshold (0.75), which is the balanced input from w_* and u_*, was proposed by Imberger (1985) and supported by field measurements (*e.g.* MacIntyre *et al.* 2002).

The energy balance can be correlated with the total net heat content (J m^{-2}) (*e.g.* Wetzel and Likens, 1991), which is given by:

$$Q_t = \frac{c_p \rho_0}{A_0} \int_0^{z_m} T(z) A(z) dz, \tag{6}$$

where $T(z)$ is the temperature (°C) at a height z (m) from the bottom. The energy budget between the maximum and minimum total net heat contents (*i.e.* $q_{t\max}$ is the maximum of $A_0 Q_t$ and $q_{t\min}$ is the minimum of $A_0 Q_t$) represents the stored energy in a water body during the one typical mixing cycle each year. A widely accepted quantity that expresses the change in seasonal heat content is the Birgean heat budget (J m^{-2}) (Hutchinson 1957), given by:

$$B_h = \frac{q_{t\max} - q_{t\min}}{A_{\text{med}}}, \tag{7}$$

where A_{med} is the mean surface of the lake (m^2). B_h is a useful indicator for describing the seasonal trend of thermal dynamics in a lake. Ambrosetti and Barbanti (2002) derived the empirical relationship between B_h and z_m: $\log_{10}(B_h) = 0.451 \cdot \log_{10}(z_m) - 0.0015 \cdot z_m + 4.98$, by studying the annual change in heat content with respect to maximum depth among ~30 lakes measured in the field.

Supplementary II

PRINCIPAL COMPONENT ANALYSIS (PCA) AND PARTIAL CORRELATION

With the four variables ($\vec{X}_i, i$ = 1 to 4) and the standard score of their datasets (n observed data), a matrix is given as

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ x_{31} & x_{32} & \cdots & x_{3n} \\ x_{41} & x_{42} & \cdots & x_{4n} \end{bmatrix} = \begin{bmatrix} \vec{X}_1 \\ \vec{X}_2 \\ \vec{X}_3 \\ \vec{X}_4 \end{bmatrix}, \quad (8)$$

where x_{ij} indicates the ith variable for the jth observed dataset. For X, the normal sample covariance matrix is defined as

$$\mathbf{R} = \begin{bmatrix} R_{11} & R_{12} & R_{13} & R_{14} \\ R_{21} & R_{22} & R_{23} & R_{24} \\ R_{31} & R_{32} & R_{33} & R_{34} \\ R_{41} & R_{42} & R_{34} & R_{44} \end{bmatrix}, \quad (9)$$

where R_{ik} is a correlation coefficient with $\bar{x}_i$ and $\bar{x}_k$, which are the mean values for the *i* or *k* variable, provided by

$$R_{ik} = \frac{\sum_j \left(x_{ij} - \bar{x}_i\right)\left(x_{kj} - \bar{x}_k\right)}{\sqrt{\sum_j \left(x_{ij} - \bar{x}_i\right)^2} \sqrt{\sum_j \left(x_{kj} - \bar{x}_k\right)^2}}. \quad (10)$$

However, these correlation coefficients may not provide good scores for components in the PCA if one variable is indirectly controlled by the other variables in reality even though they are likely to appear independent. For example, H_{net} is indirectly affected by wind speed through sensible heat and latent heat fluxes. When computing the correlation between H_{net} and other variables (S_t ratio and h_{GAP}), the effect of wind speed should be eliminated as a background aspect (*i.e.* the third variable), which can be considered as a spurious relationship.

Therefore, to derive a substantial relationship and remove a spurious relationship between two variables, we introduced partial correlation (Guilford and Fruchter, 1973), which evaluates the degree of association between two variables, with limited use. When the correlation between $\vec{X}_i$ and $\vec{X}_k$ without the effect of $\vec{X}_\ell$ is computed, a general form of the correlation coefficient is given by:

$$R_{ik,\ell} = -\frac{R_{ik} - R_{i\ell}R_{k\ell}}{\sqrt{1-R_{i\ell}^2}\sqrt{1-R_{k\ell}^2}}, \tag{11}$$

where R_{ik}, $R_{i\ell}$, and $R_{k\ell}$ are correlation coefficients (i,k), (i,ℓ), and (k,ℓ). The original matrix $\mathbf{R}$ becomes $\mathbf{R'}$. The modified $\mathbf{R'}$ can be decomposed as $\mathbf{C}^{\mathrm{T}}\mathbf{\Lambda}\mathbf{C}$ using the eigenvalue matrix ($\mathbf{\Lambda}$) and the orthogonal coefficient matrix ($\mathbf{C}$) between the original variables and the principal components. These matrices are given by

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{bmatrix} \text{ and } \mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \text{ with } \mathbf{C}\mathbf{C}^{\mathrm{T}} = \mathbf{I} \text{ (a unit matrix).}$$

with the matrix ($\mathbf{Y}$) for principal components given by

$$\mathbf{Y} = \begin{bmatrix} \vec{Y}_1 \\ \vec{Y}_2 \\ \vec{Y}_3 \\ \vec{Y}_4 \end{bmatrix} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n} \\ y_{21} & y_{22} & \cdots & y_{2n} \\ y_{31} & y_{32} & \cdots & y_{3n} \\ y_{41} & y_{42} & \cdots & y_{4n} \end{bmatrix}$$, the linear relationship between $\mathbf{X}$ and $\mathbf{Y}$ can be written by

$$\mathbf{Y} = \mathbf{C}\mathbf{X}: \tag{12}$$

$$\begin{cases} y_{1j} = c_{11}x_{1j} + c_{12}x_{2j} + c_{13}x_{3j} + c_{14}x_{4j} \\ y_{2j} = c_{21}x_{1j} + c_{22}x_{2j} + c_{23}x_{3j} + c_{24}x_{4j} \\ y_{3j} = c_{31}x_{1j} + c_{32}x_{2j} + c_{33}x_{3j} + c_{23}x_{4j} \\ y_{4j} = c_{41}x_{1j} + c_{42}x_{2j} + c_{43}x_{3j} + c_{44}x_{4j} \end{cases}$$

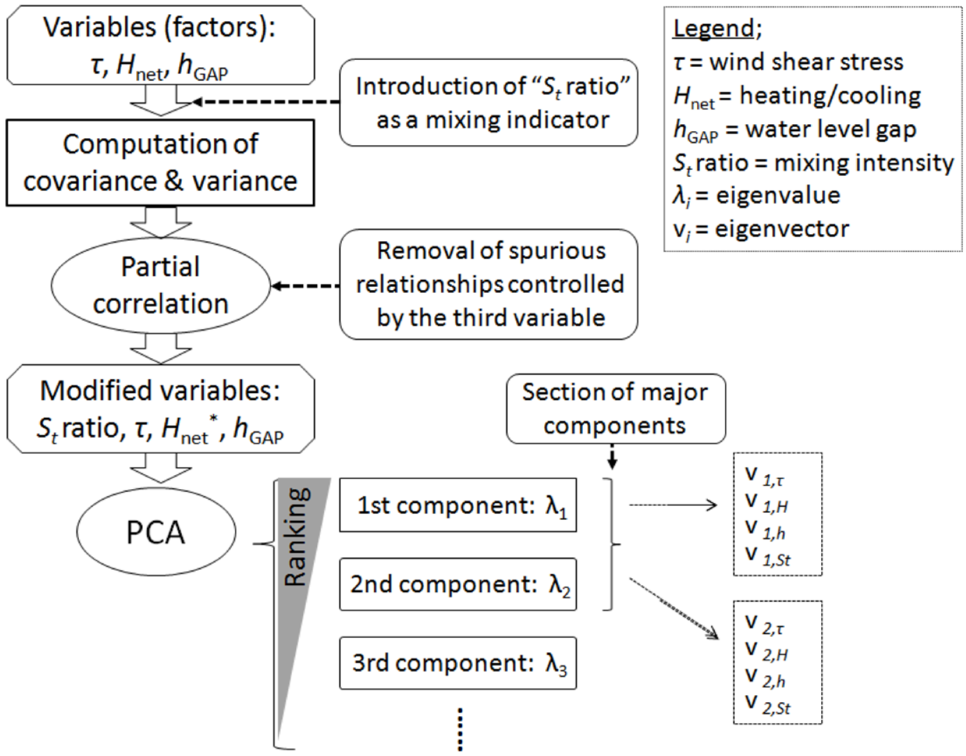
where j =1 to n. The variance of $\mathbf{Y}$ becomes

$$\mathrm{cov}(\mathbf{Y},\mathbf{Y}) = \mathrm{var}(\mathbf{Y}) = \mathbf{C'}\,\mathrm{var}(\mathbf{X})\mathbf{C'}^{\mathrm{T}} = \mathbf{C'}\left[\mathrm{E}\left(\mathbf{X}\mathbf{X}^{\mathrm{T}}\right) - \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}}\right]\mathbf{C'}^{\mathrm{T}}, \tag{13}$$

where $\mathrm{cov}(\ )$, $\mathrm{var}(\ )$, and $\mathrm{E}(\ )$ are covariance, variance and expectation respectively, and $\boldsymbol{\mu}$ is the mean (= $\mathrm{E}(\mathbf{X})$). Here, $\boldsymbol{\mu}$ =0 because $\mathbf{X}$ is described in standard score. $\mathrm{E}\left(\mathbf{X}\mathbf{X}^{\mathrm{T}}\right)$ corresponds to $\mathbf{R}$, which can be replaced with $\mathbf{R'}$. Eq. (10) then becomes

$$\mathrm{cov}(\mathbf{Y},\mathbf{Y}) = \mathbf{C}\mathbf{R'}\mathbf{C}^{\mathrm{T}} = \mathbf{C}\mathbf{C}^{\mathrm{T}}\boldsymbol{\Lambda}\mathbf{C}\mathbf{C}^{\mathrm{T}} = \boldsymbol{\Lambda}. \tag{14}$$

Thus, the principal components are mutually independent. They can consist of new orthogonal coordinates dependent on the eigenvalue vector. The relative variance scales explained by each principal component are given by $\lambda_i / \sum_i \lambda_i$ (i =1 to 4). The above procedures are shown in the flowchart (Supplementary Fig.1).



Supplementary Fig. 1. Flowchart of the procedures for the PCA and partial corrleation.