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SUPPLEMENTARY MATERIAL

Prediction of lake surface temperature using the *air2water* model: guidelines, challenges, and future perspectives

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Supplementary Material A

The net heat flux per unit surface H_{net} [Wm^{-2}] at the air-water interface (defined as positive when it is directed towards the lake) can be written as follows:

$$H_{net} = H_s + H_a + H_w + H_e + H_c + H_p + H_i + H_d, \tag{A1}$$

where

H_s is the net shortwave radiative heat flux due to solar radiation actually absorbed by the lake, H_a is the net longwave radiation emitted by the atmosphere and absorbed by the lake, H_w is the longwave radiation emitted from the lake, H_e is the latent heat flux due to evaporation and condensation, H_c is the sensible heat flux due to convection, H_p is the heat flux due to incoming precipitation, H_i is the heat exchanged with inlets/outlets, and H_d the heat exchanged between surface volume and deep water or sediments.

The last three terms are not implicitly included in the *air2water* model because of their minor effect. However, their contribution is indirectly accounted for in the calibration of parameters.

The incident solar radiation approximately follows a sinusoidal annual cycle. Considering the shortwave reflectivity r_s (albedo), which is a function of the solar zenith angle and of the lake surface conditions (*e.g.*, water wave height), the net solar radiation can be expressed as:

$$H_s(t) = (1 - r_s)\left\{s_0 + s_1 \cos\left[2\pi\left(\frac{t}{t_y} - s_2\right)\right]\right\}, \tag{A2}$$

where

t is time, t_y is the duration of a year in the units of time considered in the analysis (*i.e.*, days), and s_0, s_1, and s_2 are coefficients that primarily depend on the latitude and the shading effects due to local topography and vegetation. The effect of cloud cover is not explicitly considered in this equation.

Incoming and outgoing long-wave radiation is calculated by the Stefan-Boltzmann law, yielding to the following formulations:

$$H_a(T_a, t) = (1 - r_a)\epsilon_a \sigma (T_K + T_a)^4, \tag{A3}$$
$$H_w(T_w, t) = -\epsilon_w \sigma (T_K + T_w)^4, \tag{A4}$$

where

r_a is the longwave reflectivity, generally assumed to have a constant value (Henderson-Sellers, 1986), ϵ_a and ϵ_w are the emissivities of atmosphere and water, respectively, σ is the Stefan–Boltzmann constant (equal to 5.67x10^{-8} Wm^{-2}K^{-4}), $T_K = 273.15$ K, and T_a and T_w are the temperatures of air and water expressed in °C. Water surface behaves almost like a black body, so the emissivity ϵ_w is essentially constant and close to unity. Contrarily, ϵ_a is more variable and depends on a number of factors among which air temperature, humidity and cloud cover are the most important (Imboden and Wüest, 1995).

The latent and sensible heat fluxes are calculated through the following bulk semi-empirical relations (Henderson-Sellers, 1986):

$$H_l(T_a, T_w, t) = \alpha_l(e_a - e_w), \tag{A5}$$
$$H_c(T_a, T_w, t) = \alpha_c(T_a - T_w), \tag{A6}$$

where

α_l [Wm^{-2}hPa^{-1}] and α_c[Wm^{-2}K^{-1}] are transfer functions primarily depending on wind speed, stability of the lower atmosphere, and other meteorological parameters, e_a is the vapor pressure in the atmosphere and e_w the water vapor saturation pressure at the temperature of water (both in [hPa]). The saturated water pressure e_w can be calculated through several empirical formulas essentially depending on temperature, as for example the following exponential law:

$$e_w = a \exp\left(\frac{b\, T_w}{c + T_w}\right), \tag{A7}$$

where

$a = 6.112$ hPa, $b = 17.67$, and $c = 243.5$ °C (Bolton, 1980).

Assuming air and water temperature as the only independent variables of all flux components, equation (1) can be suitably linearized by Taylor series expansion around long-term averaged values of these variables ($\overline{T}_a$ and $\overline{T}_w$, respectively), so that H_{net} can be rewritten as in equation (2) in the manuscript, where:

$$\mathrm{H}_{net,0} = \mathrm{H}_{net}|_{\overline{T}_a, \overline{T}_w} = H_s + H_a|_{\overline{T}_a} + H_w|_{\overline{T}_w} + H_l|_{\overline{T}_a, \overline{T}_w} + H_c|_{\overline{T}_a, \overline{T}_w}, \tag{A8}$$
$$\left.\frac{\partial H_{net}}{\partial T_a}\right|_{\overline{T}_a, \overline{T}_w} = \left.\frac{\partial H_a}{\partial T_a}\right|_{\overline{T}_a} + \left.\frac{\partial H_l}{\partial T_a}\right|_{\overline{T}_a, \overline{T}_w} + \left.\frac{\partial H_c}{\partial T_a}\right|_{\overline{T}_a, \overline{T}_w}, \tag{A9}$$
$$\left.\frac{\partial H_{net}}{\partial T_w}\right|_{\overline{T}_a, \overline{T}_w} = \left.\frac{\partial H_w}{\partial T_w}\right|_{\overline{T}_w} + \left.\frac{\partial H_l}{\partial T_w}\right|_{\overline{T}_a, \overline{T}_w} + \left.\frac{\partial H_c}{\partial T_w}\right|_{\overline{T}_a, \overline{T}_w}. \tag{A10}$$

By computing, for simplicity, the 1st order Taylor expansion of equations (A1) around an unique reference temperature (i.e., $\bar{T}_a = \bar{T}_w = \bar{T}$), and substituting equations (A2)-(A7) into equations (A8)-(A10), it is easy to derive the following definitions of parameters $\hat{a}_\mathrm{i}, i = 1, 2, 3, 5, 6$ that appear in equation (3):

$$\hat{a}_1 = (1 - \bar{r}_s)s_0 + \sigma(\tilde{\epsilon}_a - \epsilon_w)(T_K + \bar{T})^3(T_K - 3\bar{T}) + \bar{\alpha}_l\left[\bar{e}_a - a\exp\left(\frac{b\bar{T}}{\bar{T}+c}\right)\left(1 - \frac{bc}{(\bar{T}+c)^2}\bar{T}\right)\right] \quad \text{(A11)}$$

$$\hat{a}_2 = 4\sigma\tilde{\epsilon}_a(T_K + \bar{T})^3 + \bar{\alpha}_c, \quad \text{(A12)}$$
$$\hat{a}_3 = 4\sigma\epsilon_w(T_K + \bar{T})^3 + \bar{\alpha}_c + \bar{\alpha}_l a\exp\left(\frac{b\bar{T}}{\bar{T}+c}\right)\left(\frac{bc}{(\bar{T}+c)^2}\right), \quad \text{(A13)}$$
$$\hat{a}_5 = (1 - \bar{r}_s)s_1 + f(r_s', \alpha_c', \alpha_l', e_a'), \quad \text{(A14)}$$
$$\hat{a}_6 = [0,1], \quad \text{(A15)}$$

where the coefficients inherently influenced by meteorological (*e.g.*, wind, cloudiness and precipitation) and astronomical phenomena (i.e., r_s, α_c, α_l, and e_a) are decomposed into a mean (indicated by an overline) and a periodic (indicated by a prime) component, and $\tilde{\epsilon}_a = (1 - r_a)\epsilon_a$.

A straightforward quantification of the parameters in equations (A11)-(A15) is not obvious since most of the physical coefficients involved do not have a single unambiguous value, but rather they can span a range of values that depends on several factors that are difficult to specify *a priori* . In particular, the definition of parameter $\hat{a}_5$ is complex, as it integrates the seasonal variability of all external forcing other than air temperature, albeit it is primarily associated with the amplitude of the annual variations of the solar radiation [see the first term of equation (A14)]. Model calibration is therefore required (see Methods section).

As a final remark, it should be noticed that after Toffolon *et al.* (2014) the notation of models parameters is slightly different than in the original paper: $\hat{a}_1$corresponding to c_3 in Piccolroaz *et al.* (2013), $\hat{a}_2$ to c_4, $\hat{a}_3$ to $c_4 - c_5$, $\hat{a}_5$ to c_1, and $\hat{a}_6$ to c_2. Furthermore, the sign of the second term of parameter $\hat{a}_1$ (i.e., c_3) was wrong in the original paper by Piccolroaz *et al.* (2013), and is now corrected in equation (A11).

Supplementary Material B

The Particle Swarm Optimization algorithm is an evolutionary and self-adaptive search optimization technique based on an iterative procedure inspired by animal social behaviour. At every iteration, the hyperspace of parameters is explored by Nparticles each one identifying a different set of parameters. The particles move within the hyperspace of parameters according to three velocity components: a spatially constant drift $\boldsymbol{v}_i^k$ (the subscript i referring to the i-th parcel, and the superscript k to the k-th iteration), and two random jumps whose amplitude depends on the current distance of the particle from the best position it explored during its movement ($\boldsymbol{p}_{best,i}^k$, where p stands for partial) and on the current distance of the particle from the best position explored in absolute by all particles before that time ($\boldsymbol{g}_{best}^k$, where g stands for global). Both bests are updated dynamically as the particles find better solutions. At each iteration k the positions $\boldsymbol{x}_i^k$ of the i-th particle is updated according to the following expression:

$$\begin{cases} \boldsymbol{v}_i^k = \omega \boldsymbol{v}_i^k + c_1 \boldsymbol{r}_1^k \left(\boldsymbol{p}_{best,i}^k - \boldsymbol{x}_i^k\right) + c_2 \boldsymbol{r}_2^k \left(\boldsymbol{g}_{best}^k - \boldsymbol{x}_i^k\right), \\ \boldsymbol{x}_i^k = \boldsymbol{x}_i^{k-1} + \boldsymbol{v}_i^k \ , \end{cases} \tag{B1}$$

where

ω is an inertia weight, which reduces the drift with the number of iterations, c_1 and c_2 are constants known as cognitive and social learning factors, respectively, and $\boldsymbol{r}_1^k$ and $\boldsymbol{r}_2^k$ are arrays of uniformly distributed random numbers bounded between 0 and 1. Note that $\boldsymbol{x}$, $\boldsymbol{v}$, $\boldsymbol{r_1}$, $\boldsymbol{r_2}$, $\boldsymbol{p}$, and $\boldsymbol{g}$ are vector having dimension equal to the number of parameters. Following the indications provided in the work of Robinson and Rahmat-Samii (2004), $c_1 = c_2 = 2$, and ω has been set to vary linearly from 0.9 at $k = 1$ to 0.4 at the final iteration. In the analysis presented here, the number of both particles and iterations are chosen equal to 1000, which showed to provide good convergence. Furthermore, absorbing wall boundary conditions are used, which means that when a particle hits the boundary of the search space, the velocity component normal to that boundary is set to zero.

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