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Vassilis Z. Antonopoulos (vasanton@agro.auth.gr)
Aristotle University

Soultana K. Gianniou
Aristotle University

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Analysis and modelling of temperature at lake's water – atmosphere interface

Vassilis Z. Antonopoulos and Soultana K. Gianniou

Department of Hydraulics, Soil Science and Agricultural Engineering,
School of Agriculture, Aristotle University, Thessaloniki 54124, Greece.
Corresponding author;
Tel: +302310 998745 ; Fax: +302310 998767; e-mails: vasanton@agro.auth.gr; tgiannio@yahoo.gr

Abstract

The knowledge of micrometeorological conditions on water surface of impoundments is crucial for the better modeling of the temperature and water quality parameters distribution in the water body and against the climatic changes. Water temperature distribution is an important factor that affects most physical, chemical and biological processes and reactions occurring in lakes. In this work, different processes of water surface temperature of lake's estimation based on the energy balance method are considered. The daily meteorological data and the simulation results of energy balance components from an integrated heat transfer model for two complete years as well as the lake's characteristics for Vegoritis lake in northern Greece were used is this analysis.

The simulation results of energy balance components from a heat transfer model are considered as the reference and more accurate procedure to estimate water surface temperature. These results are used to compare the other processes. The examined processes include a) models of heat storage changes in relationship to net radiation ($Q_t(R_n)$ values, b) net radiation estimation with different approaches, as the process of Slob's equation with adjusted coefficients to lake data, and c) ANNs models with different architecture and input variables. The results show that the model of heat balance describes the water surface temperature with high accuracy (r^2=0.916, RMSE=2.422^{o}C). The ANN(5,6,1) model in which T_{sw}(i-1) is incorporated in the input variables was considered the better of all other ANN structures (r^2=0.995, RMSE=0.490^{o}C). The use of different approaches for simulating net radiation (R_n) and $Q_t(R_n)$ in the equation of water surface temperature gives results with lower accuracy.

Keywords: Heat transport; water – atmosphere interface; energy balance components; net radiation; heat storage; ANN models

1. Introduction

The heat flux near the water-atmosphere interface, of lakes and wetlands, plays a central role in hydrology. The water temperature near the interface controls the partitioning of available energy into latent and sensible heat fluxes into atmosphere (Parlange et al. 1998). In addition, biological processes such as microbial activity and algae growth depend on the temperature status of the water profile. The water and energy balances are linked at earth/water – atmosphere interface through the evaporation. An increased interest has been about the water temperature and heat fluxes at water – atmosphere interface during the last decades due to climate change. Studies on climate change and lakes characteristics demonstrate that lakes are highly sensitive to climate, and their physical, chemical and biological properties respond rapidly to climate-related changes (Arhonditsis et al., 2004; Adrian et al., 2009). Temperature is also one of the most important driving variables for models simulating chemical and biological parameters in lakes. There are in fact several reasons to search for a reliable tool to estimate the dependence of water temperature on the various factors influencing the heat balance of lakes.

Free-surface evaporation and sensible heat transfer are mainly driven either by the vapor pressure gradient between the water surface (at temperature T_s) and the nearby surrounding air (at temperature T_a) or the difference between water surface and nearby air temperature. This implies that the knowledge of T_s is a prerequisite for the calculation of the energy budget and evaporation rates.

Micrometeorological models are able to estimate water and near-water temperatures in lakes and wetlands from air temperatures gauged by standard meteorological stations. These temperatures could significantly improve the accuracy and realism of lake's water quality models and consequently the performance of operational productivity simulation models currently used for water quality management of lakes.

Burba et al. (1999a,b) presented an analysis of surface energy fluxes of Phragmites australis in a prairie wetland. The Bowen ratio (energy balance method) was used to calculate sensible and latent heat fluxes. Confalonieri et al. (2005) presented two micrometeorological models for the simulation of thermal profile related to water and near water temperatures in flooded rice fields. The mechanistic model is based on the solution of the equation of the surface energy balance and the empirical one is funded on Gaussian filters. Both the models need as input data only daily values of

maximum and minimum temperatures and therefore are suitable for agroecological operational purposes. Duan and Bastiaanssen (2015) presented a new empirical procedure for estimating intra-annual heat storage changes in lakes and reservoirs using data from 22 lakes around the world. Duan and Bastiaanssen, (2017) evaluated a derived heat storage changes hysteresis model in the energy balance-based evaporation models to yield good evaporation estimates. Three energy balance-based evaporation models were evaluated for five different lakes at the monthly timescale where reliable reference evaporation from either the Bowen Ratio Energy Budget (BREB) or direct Eddy Covariance (EC) measuring methods were obtained from published literature. Aschonitis and Antonopoulos (2008) presented a study of heat transfer components of the paddy-rice fields using a modification of the GLEAMS-PR model and field data. Ito and Momii (2021) studied the contribution of meteorological factors to lake evaporation (E) with comprehensive analyses of lake surface temperature (T_s) under different climate scenarios.

One of the most important water impoundments in Greece is Lake Vegoritis. It has suffered from several environmental problems since the decade of 50s due to heavy industrial and agricultural pollution in its catchment area, a negative trend in the water balance and due to natural reasons as well (Gianniou and Antonopoulos, 2007a,b).

In this paper, micrometeorological approaches are used to estimate water and near-water temperatures in lakes from air temperature and heat budget components. The heat transport model (QUALAKE model) is been used to produce results which then are used to check the other procedure (Antonopoulos and Gianniou, 2003; Gianniou and Antonopoulos, 2007a). Meteorological data and water temperature and energy balance results of model simulation in Vegoritis Lake in northern Greece are used in analysis and modeling presented in the current article.

2 Mathematical descriptions

2.1 Lake water temperature modeling

The thermal content of a lake and the water temperature distribution can be determined using mathematical models. The mathematical model QUALAKE is a one-dimensional, eddy diffusion, finite element, water quality prediction model which was developed to simulate the seasonal temperature cycle, oxygen distribution and productivity for Lake Vegoritis as well as its evaporation and heat budget (Antonopoulos and Gianniou, 2003; Gianniou and Antonopoulos, 2007a,b; 2014).

The heat transport is based on the vertical diffusion equation of the form (Henderson-Sellers, 1984; Chapra, 1997; Gianniou and Antonopoulos, 2007a,b):

$$\frac{\partial T}{\partial t}=\frac{1}{A}\frac{\partial}{\partial z}(KA\frac{\partial T}{\partial z})-\frac{1}{A\rho_w c_{pw}}\frac{\partial(Aq)}{\partial z} \quad (1)$$

where K is the eddy diffusion coefficient (m^2day^{-1}), q(z) is the internal distribution of heat sources due to solar radiation absorption inside the water column (MJ $m^{-2}day^{-1}$), ρ_w is the water density (=1000 kg m^{-3}), c_{pw} is the specific heat of water (MJ $kg^{-1}{}^{o}C^{-1}$), A(z) is the horizontal area as a function of depth (m^2) and T(z,t) is the water temperature (^oC).

The mathematical model QUALAKE, was developed to study the water quality, evaporation and energy budget of lakes and specifically Lake Vegoritis (Gianniou and Antonopoulos, 2007a,b; 2014). It was calibrated and verified to predict water temperature, chlorophyll-a and dissolved oxygen distribution along the depth of the lake using measurements for two different years (Antonopoulos and Gianniou, 2003; Gianniou and Antonopoulos, 2014). The model results, during calibration and recalibration using measured data of water temperature profiles for two different years, showed (Gianniou and Antonopoulos, 2014) that there was good agreement between simulated and measured values of water temperature at different depths in the lake and on different days of the years. The values of RMSE ranged from 0.42 to 1.84 ^oC for the different water temperature profiles.

2.2 Water surface energy balance

The energy budget is based on the conservation of energy law, which accounts for incoming and outgoing energy balanced by the amount of energy stored in the system. The energy budget of a lake can be expressed as (Bowie et al., 1985; Sturrock et al., 1992):

$$Q_t = R_s - R_{sr} + R_a - R_{ar} - R_{br} - H - LE \quad (2)$$

where Q_t is the change in the energy (thermal) content of the water body, R_s and R_a are the short-wave radiation incident to water surface and the incoming long-wave radiation from the atmosphere respectively, R_{sr} and R_{ar} are the reflected short-wave and long-wave radiation respectively, R_{br} is the back (long-wave) radiation emitted from the body of water, H is the energy conducted to or from the body of water as sensible heat, and LE is the latent heat flux (due to evaporation),.The units used for the terms of Eq. (1) are MJ $m^{-2}day^{-1}$.

The water surface energy balance (Schelde et al., 1998; Colfalonieri et al., 2005; Gallego-Elvira et al., 2010) can be also described by:

$$Q_t = R_n - H - LE \quad (3)$$

In this equation R_n is the net radiation, which is described as:

$$R_n = R_s - R_{sr} + R_a - R_{ar} - R_{br} = (1-\alpha_s)R_s + (1-\alpha_a)R_a - R_{br} \quad (4)$$

where α_s is the reflectivity of short-wave radiation of water surface (α_s=0.07) and α_a is the reflectivity of long-wave radiation (α_a=0.03).

The energy utilized for evaporation (LE) and the sensible heat flux (H) can be simplified with the following approaches. The latent heat flux is as:

$$LE = \rho_w \lambda E \quad (5)$$

in which λ is the latent heat of vaporization of water (MJ kg^{-1}) and E is the water evaporation (mm day^{-1}). Latent heat of vaporization depends on water temperature according to (Allen et al., 1998):

$$\lambda = 2.501 - (2.361 \times 10^{-3})T \quad (6)$$

where T is the water temperature (^oC).

The equation of sensible heat flux (*H)* can be expressed as:

$$H = -\rho_a c_{pa} K_h \frac{\partial T}{\partial z} \quad (7)$$

where ρ_a is the density of air (ρ_a = 1.205 kg m^{-3} at 20 ^oC), c_{pa} is the specific heat of air at constant pressure (c_{pa}=1005 J kg^{-1} K^{-1}), K_h is the turbulent exchange coefficient for sensible heat (m^2day^{-1}), and $\partial T/\partial z$ is the gradient of potential air temperature. A simplification of eq. (7) is the following (Schelde et al., 1998; Antonopoulos, 2006) :

$$H = h_u(T_{sw} - T_a) \quad (8)$$

where T_{sw} is the water surface temperature (◦C), T_a is the air temperature (◦C) and h_u is the transfer coefficient of sensible heat (MJ m^{-2} d^{-1} $^oC^{-1}$), which value was expressed by Penman (1948) as a function of wind velocity with the following equation (Allen et al., 1998):

$$h_u = a_u(1 + b_u u_m) \quad (9)$$

where a_u and b_u are empirical coefficients. The values of a_u = 0.64 MJ m^{-2} d^{-1}◦C^{-1} and b_u =0.5 sm^{-1} with u_m the wind speed measured at 2 m height were suggested by Allen et al.(1998). In this study the values of a_u and b_u , adjusted to the local conditions of Lake Vegoritis are a_u = 0.25 MJ m^{-2} d^{-1}◦C^{-1} and b_u =0.54 s m^{-1}.

The flux of sensible heat (H) is related to the evaporative heat flux (LE) through the Bowen ratio (β) (Henderson-Sellers, 1984):

$$\beta = \frac{H}{LE} = \gamma \frac{T_{sw} - T_a}{e_{sw} - e_d} \quad (10)$$

where e_{sw} is the saturation vapor pressure at the temperature of the water surface (kPa), e_d is the air vapor pressure above water surface (kPa) and γ is the psychrometric constant (in kPa$^oC^{-1}$).

Combination of Eqs. (3) and (10) results in the following equation for evaporation estimation:

$$\mathrm{LE} = \frac{\mathrm{R_n} - \mathrm{Q_t}}{(1+\beta)} \tag{11}$$

Substituting in equation (3), equation (8) and rearranging the terms (Confalonieri et al., 2005) we obtain:

$$T_{sw} = \mathrm{T_a} + \frac{R_n - LE - \mathrm{Q_t}}{h_\mathrm{u}} \tag{12}$$

2.3 Heat storage and flux to the water column

The energy balance combination method for estimating evaporation and lake surface temperature requires the knowledge of heat storage changes (Q_t). The change in the thermal content of the water body (Q_t) can be determined by the change of the lake's temperature for the time step of the application of the energy budget method (day in this case) (Gianniou and Antonopoulos, 2007a), according to the equation:

$$Q_\mathrm{t} = \frac{\rho_\mathrm{w} c_\mathrm{pw}}{A_\mathrm{s}} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^{z_\mathrm{max}} A T \mathrm{d}z \tag{13}$$

in which A_s is the surface area of the lake (m^2) and $T(z,t)$ is the water temperature (^oC) as a function of depth (z) and time (t).

The lack of data on water temperature profiles hinders routine computation of Q_t (Duan and Bastiaanssen, 2015). In many studies of lake evaporation estimation Q_t is ignored to overleap the lack of measurements. Choudhury et al. (1987), Clothier et al. (1986) observed strong relationship between the soil heat flux density and net radiation (R_n) for land surfaces. Duan and Bastiaanssen, (2015) analyzing the data extracted from literature verified relationships of $Q_t(R_n)$ for each of 22 lakes they examined. Burda et al. (1999a) estimated Q_t using a linear empirical equation of R_n. The same form of empirical equation was used by Confalonieri et al. (2005) to estimate Q_t in flooded rice environment.

Quantifying approaches were developed to find a relationship between heat storage changes and net radiation (Duan and Bastiaanssen, 2015). A hysteresis model based on the rate of change of net radiation, dR_n/dt, for approximating Q_t in lakes was used as:

$$Q_t = a\, R_n + b + c\, dR_n/dt \tag{14}$$

where dR_n/dt is the rate of change (or time derivative) of R_n. The term dR_n/dt is used to account for the hysteresis-caused deviations from (or deviations that could not be explained by) the linear model ($Q_t = a\, R_n + b$).

Duan and Bastiaanssen (2015) analyzed the relationship $Q_t(R_n)$ with data from 22 lakes. The hysteresis function (eq. 14) fits the 22 independently gathered datasets satisfactory (R^2 of 0.83 and RMSE of 22 W m^{-2}) for bi-weekly and monthly time scales. They proposed for Vegoritis Lake the equations:

$$Q_t = 1.25\ R_n - 100.25 + 41.94\ dR_n/dt \qquad (r^2=0.88,\ RMSE=37.1\ W\ m^{-2}) \qquad (15a)$$

$$Q_t = 0.87\ R_n - 52.58 + 45.66\ dR_n/dt \qquad (r^2=0.92,\ RMSE=19.6\ W\ m^{-2}) \qquad (15b)$$

Using the daily results of Q_t and R_n computed by the QUALAKE model for Vegoritis lake from February 2003 to January 2005, a numerical calculation of dR_n/dt and the statistically best fitting regression model for an equation of $R_n(t)$ similar to eq. (14) was estimated as it will presented later in "results and discussion" section.

2.4 Other approaches of Net radiation and Heat budget components

Since the procedure to estimate Q_t is based on R_n and there are not any instruments to measure R_n (either satellites or land surface instruments) empirical or semi-empirical methods have been developed to estimate R_n. In the most of them shortwave solar radiation (R_s) is the drive parameter. R_s can be estimated accurately also from satellite data (Pinker et al., 1995) or semi-empirical (as Hargreaves method), Artificial Neural networks (ANN) technology and multi-linear regression methods (MLR) (Antonopoulos et al., 2019). Various other methods for computing R_n for land surfaces were recently reviewed (Kjaersgaard et al., 2009).

In the current study we investigated the performance of the Slob's equation for open water bodies. The Slob's equation was first developed for grasslands in the Netherlands (De Bruin, 1987; De Bruin and Stricker, 2000). The equation is described as:

$$R_n = (1-a)R_s - a_{slob}\frac{R_s}{R_{ex}} \qquad (16)$$

where α is the albedo of water (usually taken as 0.07, R_{ex} is the extraterrestrial atmospheric radiation and a_{slob} is the regression coefficient for net longwave radiation (MJ $m^{-2}day^{-1}$). The original value for the empirical coefficient in the Slob's equation for grasslands was a_{slob} = 9.48 MJ $m^{-2}day^{-1}$ (110 W m^{-2}) (De Bruin, 1987). The value of a_{slob} ranged from 85 to 143 W m^{-2} under different natural ecosystems and climate regimes (Duan and Bastiaanssen, 2015).

2.5. Artificial neural networks

The artificial neural networks are non-linear models that make use of a structure capable to represent arbitrary complex non-linear processes that relate the inputs and outputs of any system

(Jain et al., 2008; Diamantopoulou et al., 2011; Kisi et al, 2015; Antonopoulos et al., 2016; Zhang et al., 2017; Antonopoulos and Antonopoulos, 2017). The basic unit in an ANN is the neuron (node). Neurons are connected to each other by links known as synapses, associated with each synapse there is a weight factor.

The ANN architecture is defined by the way in which the neurons are interconnected. The network is fed with a set of input-output pairs and is trained to reproduce the output. The structure of each ANN is represented as (*i*, *j*, *k*), where *i* expresses the number of nodes in the input layer, *j* the nodes in the hidden layer and *k* the nodes in the output layer. There is a wide variety of algorithms available for training a network and adjusting its weights (Premalatha and Vala Arasu, 2016). In this article, an algorithm of the multi-layer feed forward artificial neural networks and of the back-propagation for optimization was used. The main task in developing an ANN model is to identify the input variables and the optimal network structure in order to produce the desired output accurately.

A typical structure of a multi-layer ANN model, as example, ANN (4-5-1) structure is presented with 4 variables (T_a, RH, u_2, Rs) in the input layer, 5 nodes in the hidden layer and 1 node (T_s) in the output layer.

There is no established methodology for the selection of the appropriate network architecture before training (Jain et al., 2008; Wu et al., 2014; Antonopoulos and Antonopoulos, 2017). In this study, the number of hidden neurons was identified by various trials. The trial and error procedure showed that when the number of neurons in the hidden layer is between 4 and 6 similar results are produced. As Maier et al. (2010) noted, it is not possible to draw any conclusion as to which architecture model should be used in particular circumstances and little effort has been directed into the area of network structure of ANN models development process. Details of ANN models selection and the procedure that was followed in this study have been presented at Antonopoulos et al. (2016; 2019) and Antonopoulos and Antonopoulos (2017).

2.6 Results evaluation

The quantitative procedures of model evaluation consisted of the use of the statistical analysis to calculate the root mean square error (RMSE) and coefficient of determination (r^2) between the measured and simulated values. These relationships have the form (Loague and Green 1991).

$$\mathrm{RMSE} = \left[\sum_{i=1}^{n} (P_i - O_i)^2 / n \right]^{1/2} \tag{17}$$

$$r^2 = \left\{ \left(\sum_{i=1}^{n} (O_i - \overline{O})(P_i - \overline{P}) \right) / \left(\sum_{i=1}^{n} (O_i - \overline{O})^2 \sum_{i=1}^{n} (P_i - \overline{P})^2 \right) \right\}^2 \quad (18)$$

where P_i and O_i are the simulated and measured value of water content, respectively, $\overline{O}$ and $\overline{P}$ is the mean of the measured and simulated values and n is the number of water content values. The optimum values of RMSE criteria are zero, while of r^2 is one.

2.7 Lake Vegoritis description

Lake Vegoritis is a very important natural impoundment in Greece. It is located in the northern part of Greece at northern latitude of $40^0 47'$ and at an altitude of 518 m (nowadays) (Gianniou and Antonopoulos 2014; Doulgeris et al., 2017). The surface area and the maximum depth of the lake ranged from31 to 32.1 km^2 and 39 to 40 m, respectively, in 2003-04, while the altitude, surface area and volume reached to 518 m, 47.16 $km^2$and $1207x10^6$ m^3, respectively the last period of 2015 to 2021. Lake Vegoritis appears to have significant quantitative and qualitative problems. The quantitative problems are mainly caused by lake's water usage for irrigation and to supply a number of thermo-electrical power stations and hydroelecrical demand in the area. Lake Vegoritis has been contaminated mainly with nutrients and mineral salts from industrial and urban waste of the surrounding area. The climate in the area is semi-dry, Mediterranean with two-distinguishing warm–dry and cold–wet periods during the year.

The meteorological data used for heat balance components estimations, as input in the diffusion equation of heat transfer in the lake and the evaporation estimation for Lake Vegoritis, are daily values of air temperature, relative humidity, wind speed and sunshine hours provided by two meteorological stations nearby the lake. These stations are located at the north-eastern and south-west of the lake and at a distance of one kilometre from the coast.

3. Results and discussion

Daily water surface temperature, evaporation and energy budget at the surface of Vegoritis Lake were estimated for the years 2003 and 2004 using QUALAKE model. Simulations of temperature distribution started for both years of the application on February and continued in daily time steps until the next January, because in February the water temperature distribution over the depth of the lake is considered uniform. The simulation results of QUALAKE model are considered

as reference data (they are referred in the next part of the article as reference data, e.g T_{sw} reference)

3.1 T_s estimation using heat budget components from model simulation results

In the 1st application, the lake water surface temperature (T_s) was estimated using of eq. (12) in which the heat budget components computed during the simulation of lake temperature with the QUALAKE model for Vegorits Lake. In Figure 1, the lake water surface temperature (ten days average) estimated during the temperature simulation of the lake with the QUALAKE model, the approach of eq. (12) and the air temperature from the meteorological station, for the periods of 11/2/2003 to 10/2/2004 and 11/2/2004 to 10/2/2005 are presented.

The water surface temperature is estimated with the approach of energy balance with satisfactory accuracy. It presents divergences some days from the reference data (T_{sw}) which are smoother. The statistical measurements r^2 and RMSE of T_s estimation in relation to T_{sw} are 0.916 and 2.422^{o}C, respectively. There are months with high approach of T_{sw} and months with lower approach, as the spring months. These differences during the spring months may be due to the unstable conditions of this period and the difficulties in approach of Bower ratio. The average water surface temperatures for the two year of the simulation are 15.07 and 13.86^{o}C for T_s and T_{sw}, respectively.

In a study of Livingstone and Lotter (1998) in lakes of Swiss Plateau they concluded that lake surface water temperature responses to air temperature more faithfully during periods of increasing air temperature (when the epilimnion is thin and thermal stability suppresses mixing) than during periods of decreasing air temperature (when convective mixing is deepening the epilimnion). This implies that the relationship between lake surface water temperature and air temperature is generally stronger during early summer (June, July) than during late summer (August). From Figure 1 it is obvious that similar behavior between the air and water surface temperature could be observed for Vegoritis lake.

3.2 Multilinear regression models (MLR) for estimation of Q_t and T_s.

A multilinear regression was applied to find a relationship between heat storage changes (Q_t) and the net radiation (R_n) using the 2 years daily data of Vegoritis Lake. The following equations were developed:

$$Q_t(t) = A_{QI} + 0.817026R_n(t) - 0.00726653(dR_n/dt) \qquad (r^2=0.752) \qquad (19)$$

$$Q_t(t) = A_{QII} + 0.803878\, R_n\,(t) - 0.0587375\, R_n(t-1) \qquad (r^2=0.759) \qquad (20)$$

In these equations the constant A_Q takes values ranging from -2 to -8. The higher values are during the warm days (from June 21 to September 30), the lower values during the cold days (from January 15 to February 28) and the mild values during the days of spring and autumn.

In Figure 2 the scatter diagrams between Q_t estimated with MLR models (eq.19 and 20) and Q_t derived from the data are presented. The relation is very strong with r^2 of 0.752 and 0.759 respectively for the two MLR models of eqs (19) and (20).

In Figure 3 Q_t estimated with the models MLRI (eq.19) and MLRII (eq.20) in relation to Q_t values of the energy budget at water surface using the reference data is presented. The values of Q_t estimated with the two multilinear regression models present lower variation in relation to the reference data. The maximum and minimum values are 22.07 and -21.73 (data), 19.17 and -12.68 (MLRI) and 14.87 and -9.17 (MLRII), respectively.

In Figure 4 a comparison of monthly average Q_t values estimated with the two models (eq. 15a, Qt-DB1 and eq.15b Qt-DB2) proposed from Duan and Bastiaanssen (2015 and 2017) versus Q_t values of the energy budget from QUALAKE model simulations and the monthly average net radiation for the years 2003-04 and 2004-05 is presented. The r^2 and RMSE of the two models of Duan and Bastiaanssen (2015, 2017) are 0.842 and 0.70 and 40.33 Wm^{-2} and 74.04 Wm^{-2} respectively. These values are slightly worse from the Eqs (19) and (20).

In Figure 5 the lake water surface temperature (T_s) estimated with the heat budget approach (eq. 12) using the three different approaches for Q_t estimation is presented for the period of 11/2/2003 to 10/2/2005. The maximum and minimum values of T_{sw} are 26.07, and 3.59 (data), 40.43 and -18.98 (MLRI) and 40.80, and -12.39 (MLRII), respectively. The statistical criteria values with these approaches are presented in Table 1.

3.3 R_n evaluation using different approaches

The Slob's equation for estimation R_n contains a coefficient that was estimated for specific locations. This equation was modified by adjusting the coefficient to obtain better comparison with R_n values using the data of R_n, R_s and R_{ex} from the meteorological station near Vegoritis lake. The modified equations are as:

$$RnSlob1=(1-a)R_s-13.057(R_s/R_{ex}) \qquad (r^2=0.257) \qquad (21)$$

$$RnSlob2=(1-a)R_s-7.796(R_s/R_{ex})-3.118 \qquad (r^2=0.539) \qquad (22)$$

The maximum, minimum and average values of R_n estimated with the two modified Slob's equations are 20.48, 21.54; -0.56, -2.27 and 7.41, 7.01 MJ $m^{-2}day^{-1}$, respectively for eq. (21) and (22).

Figure 6 presents the T_{sw} values (10 days average) estimated using the heat budgetcomponents in which R_n was computed using the two adjusted Slob's equations, as they are described by eqs (21) and (22), respectively. In Table 2 the statistical criteria of three models are presented.

3.4 Results of ANN models

The architecture of the ANN model was identified by the trial and error procedure (Antonopoulos and Antonopoulos, 2017). The structure of ANN models which was chosen to derive in this application contain 4 or 5 neurons in the input layer, 6 neurons in the hidden layer and 1 neuron in the output layer which corresponds to the water surface temperature estimated with the QUALAKE model, using a sigmoid transfer function. Before training and testing, the variables (T_a, RH_a, u_2, R_s) were standardized and were used as input variables. The target output variable T_s was also standardized before training and testing.

The input and output data sets were standardized by

$$y=0.9(x-x_{max})/(x_{max}-x_{min})+0.1 \qquad (23)$$

where y is the normalized value, x is the value to be normalized and x_{max}, x_{min} are the maximum and minimum values of the related value, respectively. The most accurate ANN model was selected based on the minimum value of RMSE and the maximum value of r.

The 365 daily data of the period 11/2/2003 to 10/2/2004 and the 365 daily data of the period 11/2/2004 to 10/2/2005 were employed for training and testing these models. Five cases of input variables were examined: 1) four (4) input variables (T_a, RH_a, u_2, R_s), 2) five (5) input variables (T_a, RH_a, u_2, R_s, T_s(i-1)), 3) five (5) input variables (T_a, T_a(i-1),RH_a, u_2, R_s), 4) five (5) input variables (T_a, RH_a, u_2, R_s, R_s(i-1)) and 5) three (3) input variables (T_a, u_2, R_s) and (T_a, RH_a, R_s). The target variable is T_{sw} estimated with the simulation of temperature distribution in the lake using QUALAKE model. For each case the daily data of the period 11/2/2003 to 10/2/2004 was used for training and for testing and the daily data of the periods of 11/2/2003 to 10/2/2004 and 11/2/2004 to 10/2/2005 was employed for testing, respectively. In Table 3 the ANN models and the statistical criteria of each of them are presented. Two cases with limited input variables were also examined. In the 1st the input variables were T_a, u and R_s and in the 2nd T_a,RH and R_s.

Figure 7 shows the comparison of daily T_s values estimated using the ANN models and the referent T_s values estimated with the energy budget components of lake simulations. In these Figures the cases of ANN models that use as input variable a) T_a, RH, u, Rs, b) T_a, RH, u, R_s, T_s(i-1), c) T_a, T_a (i-1), RH, u, R_s and d) T_a, RH, u, R_s, R_s (i-1), the daily data of the period 11/2/2003 to 10/2/2004 for training and the daily data of the period of 11/2/2003 to 10/2/2005 for testing are presented.

The ANNs models results, when using either 4 (T_a, RH, u_2, R_s) or 5 (T_a, T_a(i-1), RH, u_2, R_s orT_a, RH, u_2, R_s, R_s(i-1)) of basic meteorological variables as input, show (Table 3) high accuracy with coefficient of determination (r^2) and RMSE ranging between 0.761 to 0.987 and 0.105 to 0.161 ^oC, respectively either the daily data of 2004 or the 2 years data of T_{sw} was used in the testing process. Adding in input variables the variable T_s(i-1), the ANN models improve the results (0.995 for r^2 and 0.029 and 0.018 ^oC for RMSE). The accuracy and statistical criteria of ANN models of (5,6,1) structure in which T_s(i-1) is incorporated in the input variables was considered the better of all other ANN structures. Introducing R_s(i-1) in the input variables, the accuracy of the results is not improved.

Using limited input variables (T_a,u and R_s or T_a,RH and R_s) the ANN results are not loosing significant in accuracy in relation to using the four basic meteorological variables (T_a, RH, u_2, R_s).

4. Conclusions

The lake's water surface temperature was estimated with a method based on energy budget components at the interface of atmosphere and water. Different approaches of energy budget components estimation were derived. The heat storage changes and the net radiation estimation were approach in different ways. ANNs modeling technique was used also to estimate the surface temperature. The reference values of lake's surface temperature were estimated with a mathematical model of temperature and energy budget simulation (QUALAKE model). Daily meteorological data and simulation results of the heat transfer model for two years (from February 1st of 2003 to January 31th of 2005) for Lake Vegoritis in the northern Greece were used.

The main conclusions are summarized as:

1) The results of energy budget components calculated with QUALAKE model was used to estimate the temperature at lake water- atmosphere interface of Vegoritis Lake for the 2 years of applications. The daily T_s presents the same variation of T_{sw} (reference data) during the year, but it presents some oscillations around T_{sw}, which are higher during the period of January to May. It approaches with high accuracy T_{sw} the other months. The coefficient of determination (r^2) is 0.916 and RMSE is 2.42 ^oC.

2) The heat storage changes were estimated with the QUALAKE model simulations and then relationships between the daily heat storage changes and net radiation were derived. The last were then used to estimate the surface temperature with the energy balance approach. The two MLR models present high correlation between Q_t and R_n (r^2 near to 0.75). The linear correlation of $Q_t(R_n)$ functions show slopes of 0.64 and 0.85, which explain why the proposed models underestimate the values of Q_t at the high positive and negative values of R_n. In monthly basis Q_t values show the hysteresis that was observed by Duan and Bastiaanssen (2005) in relation to R_n values. T_s values calculated with the MLR models show intensive oscillations during the year. There are days with very high or very low surface temperature, which could not be explained because they are not in agreement with the values of of reference data (T_{sw}).

3) The net radiation was estimated with different approaches, as the Slob's equation. The coefficient of Slob's equation was adjusted to the local conditions and the data of Vegoritis lake. These approaches were used then in the process of surface temperature estimation. Two models of Slob's equation were adjusted to local conditions. The one model in which a constant term was added show higher correlation in relation to the 2nd model. T_{sw} values of heat budget components

evaluation show oscillations around the reference data. The statistical criteria are 0.639 and 0.758 for r^2 and 5.015 and 4.324 ^oC for RMSE, respectively.

4) The ANNs modeling techniques were also used to estimate the surface temperature, using different model architects. The derived ANN models of different structure showed that they could describe T_s with high accuracy. In these models 4 input meteorological variables (T_a, RH, R_s, u_2) and 5 alternative variables (T_a,(or T_a(i-1)), RH, R_s,(or R_s(i-1)), u_2 and T_s(i-1)) were analyzed. The r^2 and RMSE of examined ANN models ranged from 0.952 to 0.697 and 0.49 to 3.40 ^oC, respectively. The most accurate is that with T_a,RH,u, R_s,T_s(i-1) as input variables. The results, for the training and the test data sets clearly demonstrate the ability of the ANN models to predict very well the daily values of T_s at the interface of air-water of lakes by using daily meteorological parameters which are introduced as inputs into the chosen ANN models. The ANN models introduced in this study have the ability to develop a generalized solution and seem promising to be applicable for the prediction of daily values of T_s.

A general conclusion is that ranging the examined cases of models with different configuration, ANN models are the most accurate, followed by the models of R_n calculated using the adjusted Slob's equations and then the models with the $Q_t(R_n)$ functions. The heat storage changes (Q_t) is the crucial variable in estimating T_s. Long time data sets of Q_t should be collected either through water temperature simulation models (diffusion models) either satellite measurements.

Availability of data and materials

The datasets generated during and/or analysed during the current study are available from the corresponding author on reasonable request.

Competing interests/Conflict of interest

There is not any disclose interests that are directly or indirectly related to the work submitted for publication.

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Authors' contributions

All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by Vassilis Antonopoulos and Soultana Gianniou. The first draft of the manuscript was written by Vassilis Antonopoulos and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Conceptualization: Vassilis Antonopoulos; Methodology, Formal analysis and investigation: Vassilis Antonopoulos, Soultana Gianniou; Writing - original draft preparation: Vassilis Antonopoulos; Writing - review and editing: Vassilis Antonopoulos, Soultana Gianniou; Funding acquisition: none; Supervision: Vassilis Antonopoulos.

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Figures

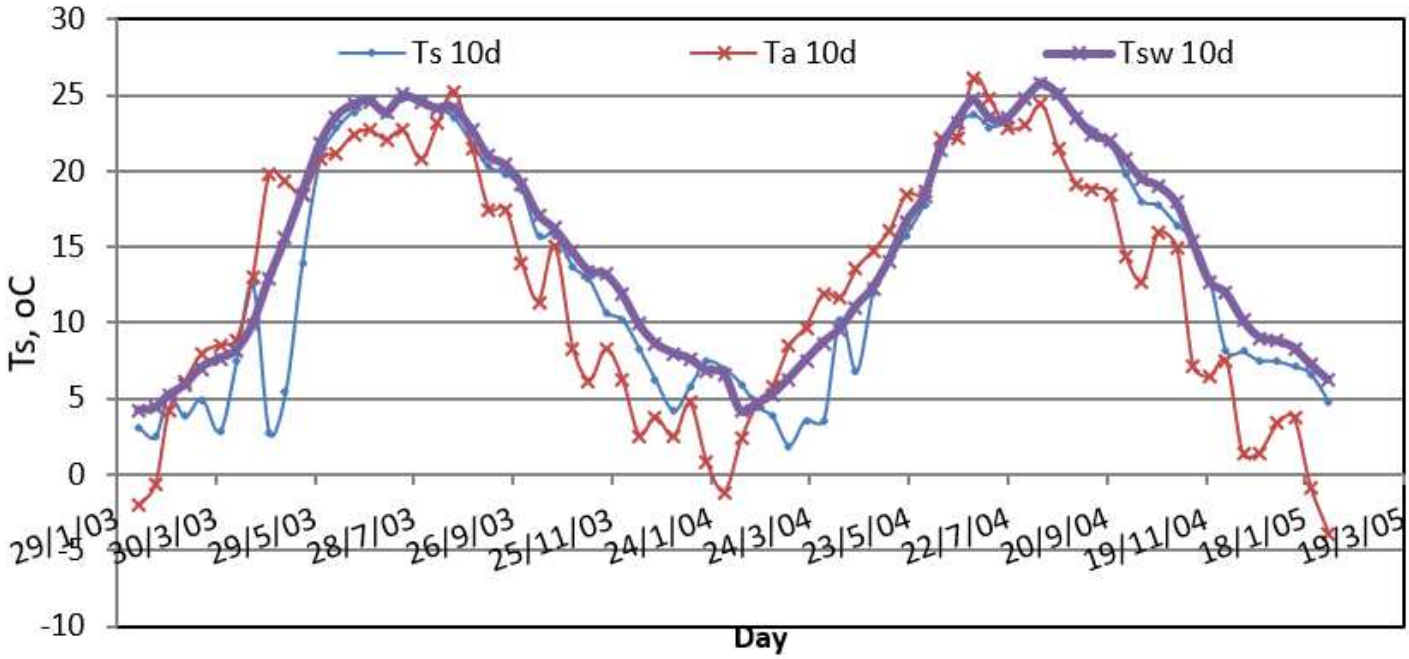

Figure 1

Comparison of Ts estimated using QUALAKE model heat budget components and eq. (12) (Ts), air temperature (Ta) and surface water temperature of the lake (Tsw) (values of Ts,Tsw and Ta are 10 days averages).

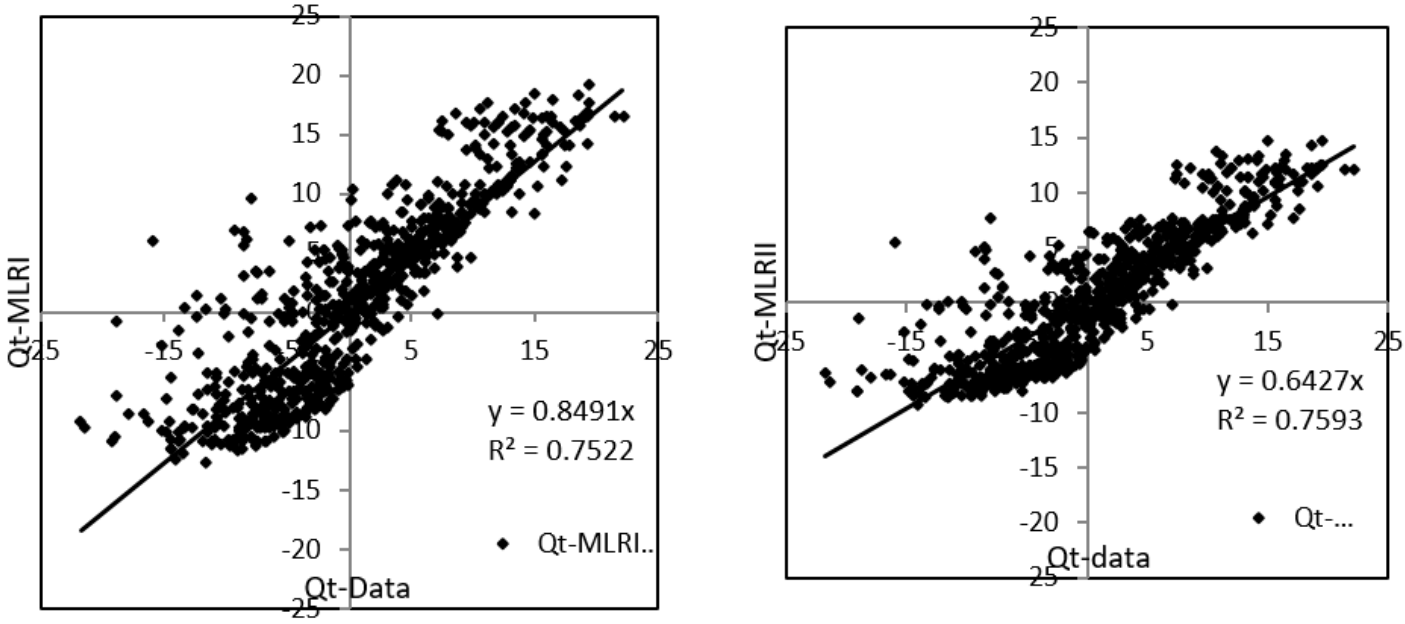

Figure 2

Scatter diagrams between Qt estimated with MLR equations (19) (MLRI) and (20) (MLRII) and Qt derived from the data.

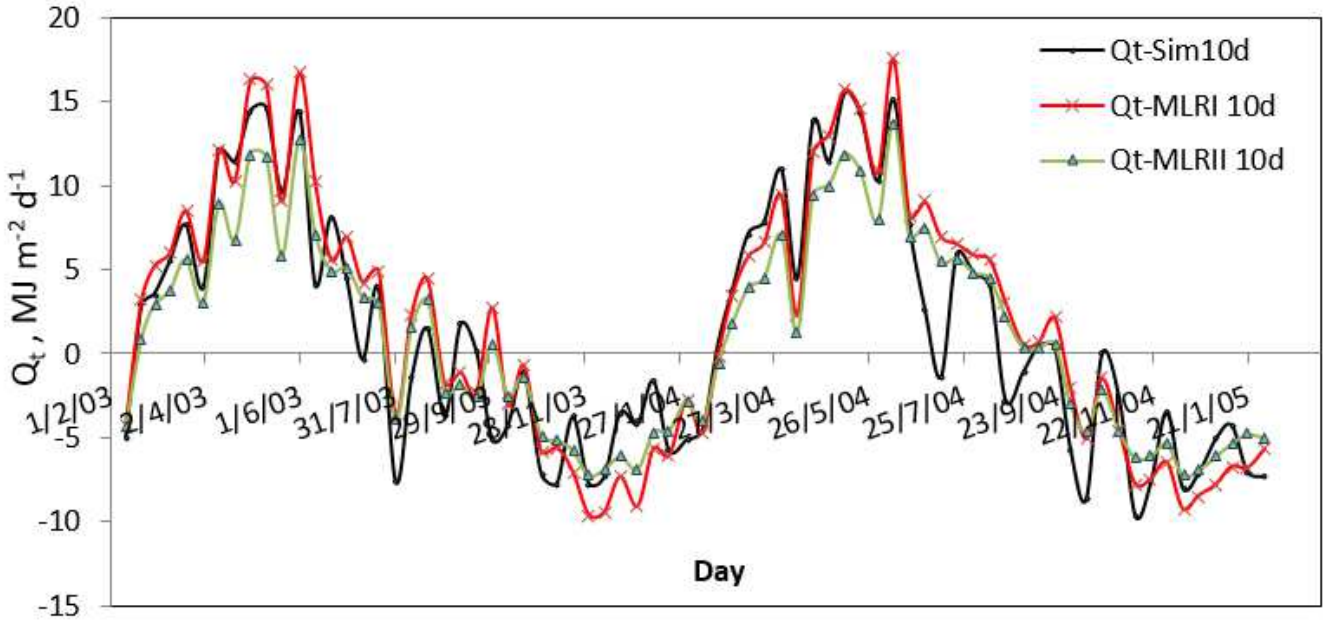

Figure 3

Comparison of Qt estimated with the two multilinear regression models (MLRI) and (MLRII) versus Qt values derived from the reference data (The values of Qt are the 10 days averages).

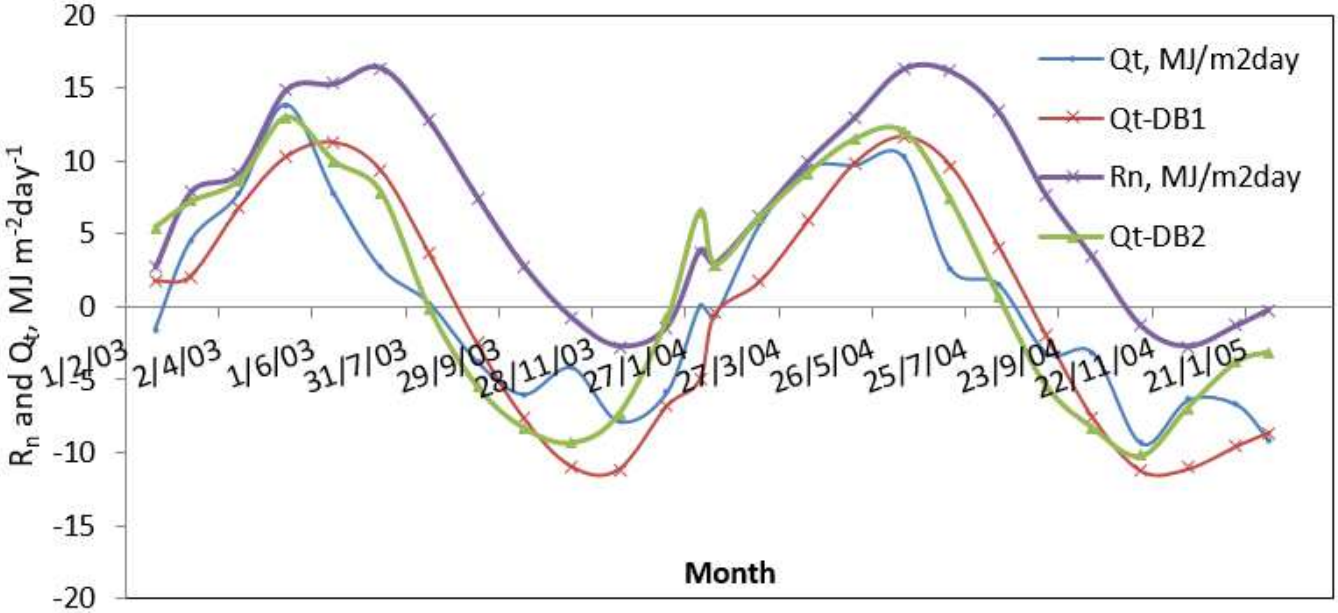

Figure 4

Comparison of monthly average Qt values estimated with the two models (Qt-DB1 and Qt-DB2) proposed from Duan and Bastiaanssen versus the Qt values of energy budget estimated by the QUALAKE model and monthly average net radiation for the years 2003-04 and 2004-05.

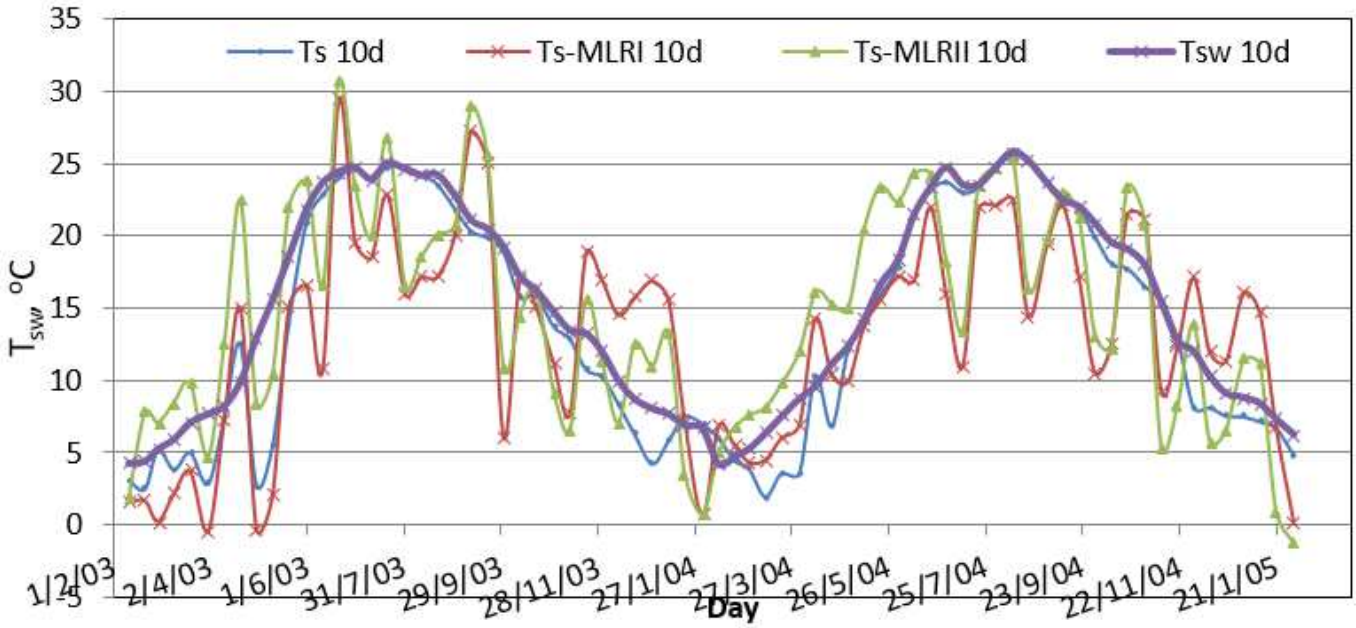

Figure 5

Lake water surface temperature using eq (12) and Qt estimated from the heat budget components and with the two different multilinear regression models Qt as function of Rn versus the results of QUALAKE model (reference data) (ten days average values).

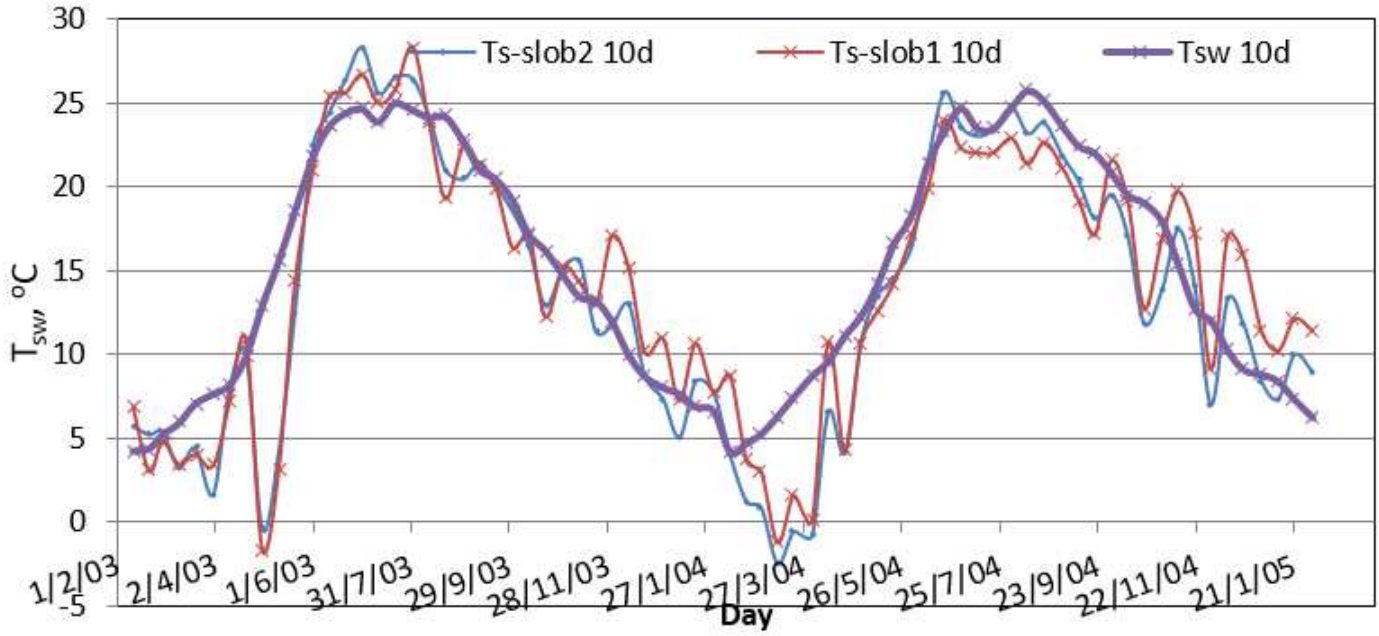

Figure 6

Comparison of Tsw estimated using the energy budget equation in which Rn was estimated using the adjusted Slob's equations to lake conditions (ten days average values).

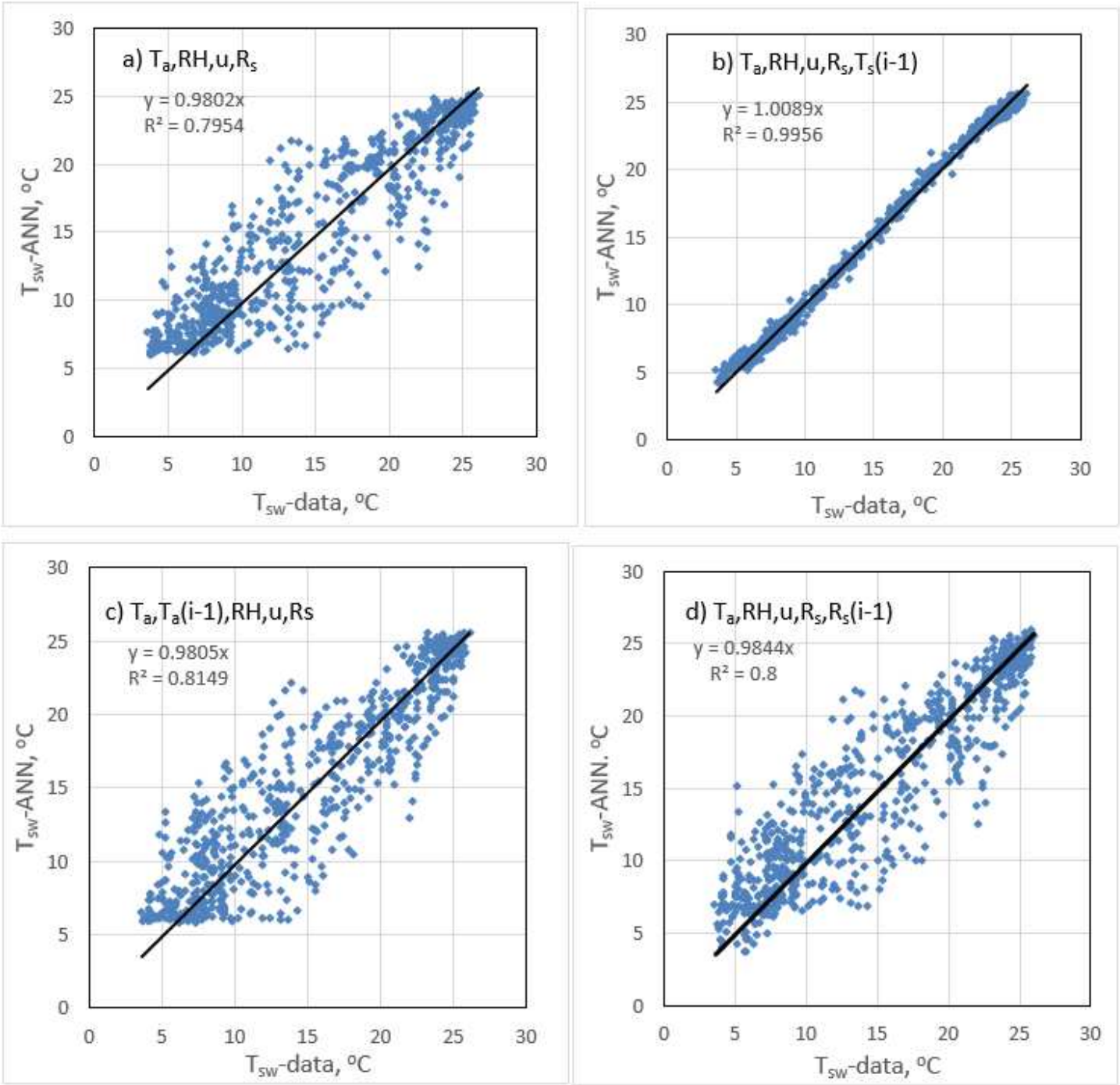

Figure 7

Scattering diagrams between water surface temperature estimated with ANN(4-6-1) and ANN(5-6-1) models in comparison to temperature estimated with QUALAKE model. In the ANN model a) four (4) input variables (Ta, RHa, u2, Rs), b) five (5) input variables (Ta, RHa, u2, Rs, Ts(i-1)), c) five (5) input variables (Ta, Ta(i-1), RHa, u2, Rs), and d) five (5) input variables (Ta, RHa, u2, Rs, Rs(i-1)), the daily data from 11/2/2003 to 10/2/2004 are used for training the model and the daily data from 11/2/2003 to 10/2/2005 are used for testing.