Numerical modeling of thermal regime in inland water bodies with field measurement data

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Abstract. Modification of the program complex LAKE, which is intended to compute the thermal regimes of inland water bodies, and the results of its validation in accordance with the parameters of lake part of Gorky water reservoir are reviewed in the research. The modification caused changing the procedure of input temperature profile assignment and parameterization of surface stress on air-water boundary in accordance with the consideration of wind influence on mixing process. Also the innovation consists in combined methods of gathering meteorological parameters from files of global meteorological reanalysis and data of hydrometeorological station. Temperature profiles carried out with CTD-probe during expeditions in the period 2014-2017 were used for validation of the model. The comparison between the real data and the numerical results and its assessment based on time and temperature dependences in control points, correspondence of the forms of the profiles and standard deviation for all performed realizations are provided. It is demonstrated that the model reproduces the results of field measurement data for all observed conditions and seasons. The numerical results for the regimes with strong mixing are in the best quantitative and qualitative agreement with the real profiles. The accuracy of the forecast for the ones with strong stratification near the surface is lower but all specificities of the forms are correctly reproduced.

1. Introduction
Vertical temperature distribution is one of the main characteristics of natural geophysical objects. It has a great impact on biology and ecology of inland water bodies such as lakes and water reservoirs, it significantly affects eutrophication (enrichment of a water body with nutrients). In [1-3] the influence of temperature distribution on proliferation of microorganisms is established, particularly proliferation of cyanophyta and diatoms. Due to their small size, lakes and water reservoirs are sensitive to mixing and wind-wave coupling, so the thermal regime is characterized by strong seasonal and short-term variability, which was researched in [4-6]. It should also be noted, that there is a growing number of requests for forecasts of thermal regimes in inland water bodies [7] which cannot be obtained from global meteorological forecasts.

There are different models, one- and multi-dimensional ones, which are used for computation of the hydrological parameters, such as thermal regimes of inland water bodies. Models based on one-
dimensional heat equation have fewer requirements for computing resources than multi-dimensional ones, and demonstrate satisfactory agreement with experimental evidence. On the other hand, these models require validation in accordance with the parameters of the given water body, and field measurement data are used for this purpose. One-dimensional model is submitted in the program complex LAKE, developed in [8] and used in this research. Modification of the program complex and its validation in accordance with the parameters of mid-sized lowland water bodies with an example of lake part of Gorky water reservoir (56°42'N 43°19'E) are provided. The data from the hydrometeorological stations closest to the water object and the files of meteorological reanalysis NCEP/NCAR were used for validation.

2. Model description and numerical implementation

The model is based on the one-dimensional heat equation:

\[ \frac{\partial T}{\partial t} = \frac{1}{\rho c_p h} \frac{\partial}{\partial \xi} \left( \lambda \frac{\partial T}{\partial \xi} \right) + \frac{\partial}{\partial \xi} \left( \rho h \frac{\partial T}{\partial \xi} \right) - \frac{1}{h} B_w \frac{\partial T}{\partial \xi} - \frac{1}{h} \frac{\partial S}{\partial \xi} \]  

(1)

The symbols are: \( c \) is heat capacity of the water, \( \rho \) – its density, \( \lambda \) - eddy diffusivity, \( T \) – temperature, \( B_w = dh_0/\partial t \) – water balance at free surface of lake, \( S \) - solar radiation flux penetrating the water body. The beginning of the vertical downward \( z \)-coordinate is supposed to be coupled with water surface, so we can turn from \( z \) to the new independent variable \( \xi = z/h \) where \( h = h(t) \) is a depth of water body, and \( t \) is a time.

The following generally accepted exponential relation is used for the calculation of the solar radiation flux penetrating the water body:

\[ S(\xi) = S(0) \exp(-\alpha, h\xi), \]

where \( S(0) \) is solar radiation flux on the surface of water, \( \alpha, h \) - extinction coefficient. Temperature gradient (heat flux) is a boundary condition for the equation (1) on the air-water boundary and is calculated from the equation of heat balance:

\[ S(1-\alpha) + E_a - E_s - H_s - LE_s = -\frac{\lambda \partial T}{h} \]  

(2)

where \( S \) is total solar radiation flux, \( E_a \) – longwave radiation flux, \( E_s \) – radiation of surface, \( H_s \) and \( LE_s \) are overt and covert heat fluxes respectively.

The finite-difference scheme of the equation (1) is as follows:

\[ \frac{T^{j+1}_i - T^j_i}{\Delta t} = \frac{1}{(h)^2} \frac{1}{\Delta \xi^2} \frac{\partial^2 T}{\partial \xi^2} + \frac{1}{\Delta \xi} \frac{\partial T}{\partial \xi} \]  

(3)

Indexation of nodes in difference grid is used here: superscript represents the number of timestep, and subscript – the number of node on the vertical coordinate. The system of linear equations (4) has a tridiagonal matrix and can be solved with Thomas algorithm or cyclic reduction.

Equation of heat balance (2) is used to calculate the temperature on the air-water boundary and has the following submission in difference form:

\[ E_s^* + S^*(1-A) - \delta \sigma \left( T^{s+1}_s \right)^4 - H_s \left( T^{s+1}_s, 0 \right) - LE_s \left( q^{s+1}_s, \left( T^{s+1}_s \right) \right) = -\frac{T^{s+1}_s - T^{s+1}_j}{h/A \xi}. \]

The symbols are the following: index \( s \) is the value on the surface, \( (s + 1) \) – the value of the node next to the surface, \( a \) is the value of the node on the atmosphere level where meteorological parameters are defined, asterisk * is values, which are given from field measurement data.

Eddy diffusivity \( \lambda \) is the main mechanism to describe vertical heat and mass exchange in water objects. There are different ways of its parameterization, we use parameterization based on equations of kinetic energy of turbulence and its dissipation rate, or "\( E - \lambda \)"-parameterization. \( \lambda \) is defined as follows:
\[ \lambda = c_p k, \]

where \( k \) is the coefficient of turbulence evaluated as
\[ k = C_e \frac{E^2}{\varepsilon}. \]

Here \( E = \frac{1}{2} \left[ (u')^2 + (v')^2 + (w')^2 \right] \) is kinetic energy of turbulence; the upper line is symbol of averaging, the values with primes are deviations from mean values, \( \varepsilon \) is dissipation rate of kinetic energy of turbulence, \( C_e \) is the dimensionless coefficient. This equation is used to estimate \( E \):
\[ \frac{\partial E}{\partial t} + \alpha_c \frac{\partial E}{\partial \xi} \frac{k}{\varepsilon} + \frac{\xi}{h} \frac{\partial}{\partial t} \frac{\partial E}{\partial \xi} + P - \varepsilon, \]

where \( \alpha_c \) is the dimensionless constant, and \( P \) is total generation of turbulence energy through the shear of velocity and effect of density stratification.

Dissipation rate of turbulence energy is defined with the following equation:
\[ \frac{\partial \varepsilon}{\partial t} = \frac{\alpha_c \varepsilon}{h^2} \frac{\partial \varepsilon}{\partial \xi} \frac{k}{\varepsilon} + \frac{\xi}{h} \frac{\partial}{\partial t} \frac{\partial \varepsilon}{\partial \xi} + C_1 \frac{\varepsilon}{E} (P - \varepsilon), \]

where \( \alpha_c \) is the dimensionless constant, and \( C_1 \) is the function of Reynolds number, which is defined as follows:
\[ \text{Re} = \frac{(2E/3)^2}{\nu E}. \]

To approximate the kinetic energy of turbulence equation and its dissipation rate equation, Crank-Nicolson numerical scheme is used. Equations (3–4) are replaced with the finite-difference analogues:
\[ \delta_t E_{i+1/2}^{j+1} = \frac{\alpha_c \delta t}{h_j} \delta_x \left( k_{i+1/2}^{j+1/2} \delta_x E_{i+1/2}^{j+1/2} + \frac{h_{i+1/2}^{j+1} \delta_t h_{i+1/2}^{j+1} \delta_x E_{i+1/2}^{j+1/2} + P_{i+1/2}^{j+1/2} - \varepsilon_{i+1/2}^{j+1/2} \right), \]
\[ \delta_t \varepsilon_{i+1/2}^{j+1} = \frac{\alpha_c \delta t}{h_j} \delta_x \left( k_{i+1/2}^{j+1/2} \delta_x E_{i+1/2}^{j+1/2} + \frac{h_{i+1/2}^{j+1} \delta_t h_{i+1/2}^{j+1} \delta_x E_{i+1/2}^{j+1/2} + C_{1i+1/2}^{j+1/2} \delta_x E_{i+1/2}^{j+1/2} - \varepsilon_{i+1/2}^{j+1/2} \right). \]

Boundary condition for equation of kinetic energy of turbulence on the air-water boundary is as follows:
\[ -\frac{k}{h} \frac{\partial E}{\partial \xi} = k_{we} \left( \frac{T}{\rho} \right)^3, \]

where \( k_{we} \) is coefficient of turbulence enhancement by wave breaking and \( \tau \) is surface stress. Assumption about continuity of impulse flow is used for zonal and meridional components of current velocity on the air-water boundary, and these components are computed with the theory of similarity by Monin-Obukhov, whereas these components on the boundary water-soil are defined with Chezy formula [9].

3. The data and parameters used for computation

The input parameters and data, which are recorded during all computation time, are set at the start of the program. Also meteorological data are used but they are read on the every step of computation.

The input temperature profile was defined with temperature difference between the surface and the bottom and the thickness of mixed layer in previous version. Three points were accounted: temperature on the surface, on the lower boundary of mixed layer and on the water-soil boundary. This limited the possibility of using the results from field measurements. In the modified version the input profile is arbitrary defined as a two-dimensional array of points from the file with values of temperature on every step of the depth. This modification allows to reproduce thermocline stratification typical for mid-sized lowland water bodies. The values of main physical parameters used in the model are either set through field measurement data or adjusted on the basis of correspondence between numerical results and real data. Therefore, the coefficient of solar radiation extinction in water body is set through measurements with Secchi disk drawing on the theory developed in [10]. However, the coefficient of turbulence enhancement by wave breaking is taken equal to 10 for the best
match between the forecast and the experimental evidence. Parameterization of this parameter is foreseen, and the dependence between its value and the value of wind velocity has to be determined for this purpose.

The parameters of meteorological conditions are as follows: air temperature, atmospheric pressure, specific air humidity, precipitation, zonal and meridional wind components, downward solar (shortwave) radiation and downward longwave radiation. These parameters are collected with combined method: information is taken from the data of hydrometeorological station in Gorodets and the files of global meteorological reanalysis NCEP/NCAR [11] with spatial resolution 1°. The timestep for meteodata is 6 hours. Information about wind velocity is used to compute surface stress on air-water boundary included in boundary condition for kinetic energy (5). In previous version empirical parameterization proposed in [12] was applied, but it ignored features of underlying surface:

\[ \tau = 1.273 \times 10^{-3} \times w_r \]

where \( w_r = \sqrt{u^2 + v^2} \), \( u \) and \( v \) – wind components. We use updated formula based on multi-year measurements of wind conditions on the experimental sites of Gorky water reservoir (see [13]):

\[ \tau = 1.274 \times 10^{-3} \times w_r + 3.4 \times 10^{-4} \times w_r^2 + 4.9 \times 10^{-5} \times w_r^3. \]

4. Validation and results

Field measurement data were used for validation of modified model. These data were obtained from the observations during expeditions on the experimental sites of Gorky water reservoir in the period 2014-2017. Measurement of the vertical temperature profiles were carried out with CTD-probe. Several measurements were made during every expedition, the results were averaged. 2014 and the current year were chosen from a large volume of data, because the seasons had a great difference in the thermal regimes due to the difference in seasonal meteorological conditions (see fig.1). 2014 was characterized by intensive solar radiation, a high temperature and a slightly weaker wind. So the temperature profiles obtained in 2014 were characterized by significant temperature difference and strong stratification, whereas the profiles obtained in 2017 are homogeneous in depth owing to weak heat and strong mixing.

Time and temperature dependences in control points (surface, 1 meter and 8 meters) were reviewed to analyze numerical results. More of points are taken closer to the surface than to the bottom, because this layer is more exposed to variability and has a significant impact on eutrophication.

![Figure 1](image1.png)  
Figure 1. Average daily values of a) solar radiation, b) air temperature, c) wind velocity in 2014 and 2017.
It is evident that the greater the depth, the less the difference is. It confirms that variability and complexity of processes are greater near the surface due to wave-wind coupling. Also the forms of profiles were compared (see fig. 3). Numerical simulation reproduces general forms of distribution for all realizations. However, the best agreement is obtained for the regimes with strong mixing, when stratification is practically nonexistent.

As for the integral characteristics of comparison between the real data and the model results, standard deviation does not exceed 0,8°C for all performed realizations for 2017 year, and 1,5°C for 2014 year, which is more accurate than the results in the previous version [8].

5. Conclusion
Modification of the program complex LAKE, which is proposed in [8] and intended to compute the thermal regimes, and the validation of the complex in accordance with the parameters of mid-sized lowland water bodies with an example of Gorky water reservoir were realized. The modification caused changing the procedure of input data assignment and led to greater consideration of wind influence on mixing. The combined method was used for validation: field measurement data, files of global meteorological reanalysis and data of hydrometeorological station were used. Numerical
simulation with the modified model gives results which are in good agreement with the real seasonal variations of thermal regime in lake part of Gorky water reservoir.

However, regimes with strong mixing and weak heat are reproduced more accurately, than regimes with strong heat and stratification, so the model results for 2017 match the field measurement data better, than the model results for 2014. The results were obtained with the same physical parameters. It can be explained by not quite adequate simulation of processes with weak wind and intensive solar radiation or by incorrect meteorological data, particularly data from reanalysis by reason of coarse grid.

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