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On the numerical performance of turbulent closure schemes in a 1D lake model

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Abstract. The turbulence closure is a crucial part of a lake model. The closures commonly used are different in underlying physics and mathematical properties, leading to contrasting numerical stability and computational efficiency. We tested the performance of the one-dimensional model LAKE using the $k - \epsilon$ closure and Henderson–Sellers turbulence parameterizations, with a convective mixing scheme, in idealized Kato–Phillips experiment and Lake Kuivajärvi (Finland) simulations. Our results demonstrate that $k - \epsilon$ closure allows for a physically realistic solution at timesteps $\Delta t < 450$ s, and the convergence of numerical scheme is attained at $\Delta t < 100$ s. In contrast, convergence of the lake model scheme using Henderson–Sellers diffusivity is achieved if $\Delta t < 3600$ s, resulting in drastic reduction of the lake model runtime as compared to using $k - \epsilon$ parameterization. At the same time, the performance of the model involving both schemes in respect to measurements is similar.

1. Introduction

Prominent development of the computational facilities during last decades has led to continuous increase of the spatial resolution in numerical weather prediction (NWP) systems and Earth System models (ESMs). For instance, in the CMIP7 project the resolution of atmospheric models attains $0.25^\circ - 0.5^\circ$ ($\sim 25\text{--}50$ km). Concomitantly, many previously subgrid objects on the Earth's surface, such as water bodies, rivers, swamps, etc., become large-scale structures (i.e. resolved or occupying a significant fraction of the land cells) and should be represented by physically sound parameterizations.

Inland waters play an important role in the formation of local weather conditions and in many respects determine the specific features of climate over the adjacent territory. Primarily, this is due to a significant difference between the lake surface temperature and the temperature of the surrounding land. This difference is observed almost always, except for the cases when lakes and soil are covered with snow. There is a significant difference between the water bodies and land in other surface thermal and aerodynamic characteristics, such as roughness and albedo. All this leads to a significant spatial heterogeneity of the turbulent and radiation fluxes on the surface, especially in regions where the density of lakes is high, for example, the West Siberian Lowland.

The contrast in the energy fluxes at the land–water boundary has a daily cycle, leading to a local atmospheric circulation along the coast of large lakes during the ice-free period. In a temperate climate zone, the presence of large water bodies changes the heat exchange in the surface air layer on the seasonal time scale. During summer, water bodies accumulate heat from shortwave solar radiation, and during autumn they release this heat, increasing turbulent fluxes as a result of large temperature and humidity gradients between the water body surface and the overlying air [1]. The heat released



from lakes at the end of autumn and in early winter during cold air outbreaks often leads to the development of horizontal convective cells in the atmospheric boundary layer – a classic scenario comprehensively studied for the Great American Lakes [2]. These examples clearly show the importance of realistic representation of lakes in numerical weather prediction systems and in Earth system models.

In the lake parameterizations embedded into NWP and ESMs [3-7], the main focus is on the thermodynamic interaction with the atmosphere, and the dynamics (not available in all parameterizations) is used only to calculate the vertical turbulent heat exchange in the water body. The fluxes of sensible, latent heat, and momentum are the boundary conditions for atmospheric models and, therefore, reliable calculations of these variables are primarily required from the lake parameterizations. However, realistic reproduction of the vertical temperature profile in a water body is also important, since this profile is a key factor for the aquatic ecosystems, which, in turn, can affect the atmospheric processes. For instance, in the last decade considerable attention has been given to the emission of methane from inland waters, in particular, thermokarst lakes [8].

Due to computational simplicity, one-dimensional models are well suited for climate modelling where lakes have to be taken into account in thousands of grid cells and where numerical experiments are carried out for long climate timescales (centuries) [3]. Within the framework of ESMs, two requirements apply to any physical parameterization, namely, computational efficiency time steps (~1 h) and physical adequacy.

The restriction imposed on the lake model resolution, both in space and time, motivates us to investigate the sensitivity of the numerical solution to the grid step variation and its convergence. This can be done using idealized numerical experiments demonstrating the role of individual key heat exchange mechanisms in the reservoir and experiments simulating particular lakes.

2. Methodology

The lake model LAKE [9] solves the 1D heat and momentum equations resulting from horizontal averaging of 3D hydrodynamic equations; the biogeochemical module reproducing the production and emission of CH₄ and CO₂ has also been implemented [9]. Like in other $k - \varepsilon$ models, in the LAKE the turbulent thermal conductivity and viscosity coefficients are found using the Kolmogorov formula,

$$\nu = C_e \frac{k^2}{\varepsilon}, \nu_T = C_{e,T} \frac{k^2}{\varepsilon},$$

where the turbulent kinetic energy (TKE) k and its dissipation rate ε are calculated on the basis of the $k - \varepsilon$ turbulent closure. This turbulent closure is widespread in solving problems of technical and geophysical hydrodynamics. The limits of its applicability and numerical stability when included in the three-dimensional Reynolds equations were shown for geophysical flows in [10] and [11].

The model LAKE2.0 has been modified and included into the INMCM ESM [12]. For simplicity, constant depth throughout a lake was assumed. Also, a one-dimensional parameterization of the thermal conductivity coefficient [13] for stably stratified lakes was added, along with a convective mixing scheme [14].

The accuracy of the numerical solution and its convergence in $k - \varepsilon$ models is an issue, especially in the context of large time step requirements in the ESM, and using semi-implicit finite-difference schemes (e.g., the Krank-Nicolson scheme). Moreover, the Kolmogorov coefficients in the standard $k - \varepsilon$ model are set constants, which is justified for neutrally stratified flows [15]. A more physically sound approach is to consider these coefficients as functions of stratification and shear, as, for instance, in the paper of Canuto [16], and Galperin stability functions [17].

A necessary condition for the convergence of a finite-difference solution of the system of differential equations to an exact one is the vanishing to zero of the norm of the difference of finite-difference solutions with different space-time resolution as the time and space steps tend to zero. This condition will be checked in subsequent sections for $k - \varepsilon$ and Henderson-Sellers, with a convective mixing scheme, closures in the LAKE model in an idealized Kato-Phillips experiment and simulation of the Kuivajarvi Lake (Finland).

3. Kato-Phillips experiment for the $k - \varepsilon$ model

3.1. Experiment setup

An idealized wind mixing scenario is considered in the model consistent with the classical laboratory experiment [18]. In the experiment, the mixed layer induced by a constant surface stress entrains in a

stably stratified fluid with the density linearly growing down from the surface. The model simulations are compared to the mixed-layer depth dependence on time $D_m(t)$, a known theoretical approximation to laboratory data [19].

$$D_m(t) = 1.05w_s N_0^{-\frac{1}{2}} t^{\frac{1}{2}},$$

where w_s is the surface friction velocity and N_0 is the Brunt-Väisälä frequency of the initial temperature profile.

The experiment was performed with the LAKE model. A zero heat flux was set at the lower and upper boundaries. The initial temperature profile was set as a linear one:

$$T(z) = 2z + 5,$$

where the z-axis is directed opposite to the gravity vector, and the corresponding $N_0 = 5.5 * 10^{-2} s^{-1}$ is typical for the summertime thermocline in the midlatitude lakes. The initial flow velocity was set to zero and the depth was set to 20 meters, $w_s = 3 * 10^{-3} ms^{-1}$. The Coriolis parameter was assumed to be 0.

For each of the $k - \varepsilon$ turbulent closures (i.e. with Canuto and Galperin stability functions), two groups of numerical experiments were carried out (Table 1), one with a varying time step Δt^k and with a fixed vertical resolution, M levels, and the second with a variable vertical resolution, M^k , and a fixed time step Δt .

Table 1. Spatial and temporal resolution in two groups of numerical experiments.

Experiment name	Fixed parameter of spatial/temporal resolution	Variable parameter of spatial/ temporal resolution	Experiment index range
<i>Gr. 1.k</i>	$\Delta t = 25 s$	$M^k = 10; 20; 40; 80; 160; 320; 640,$	$k = 1..7$
<i>Gr. 2.k</i>	$M = 40$	$\Delta t^k = 3600; 1800; 900; 450; 225; 100; 50; 25 s$	$k = 1..8$

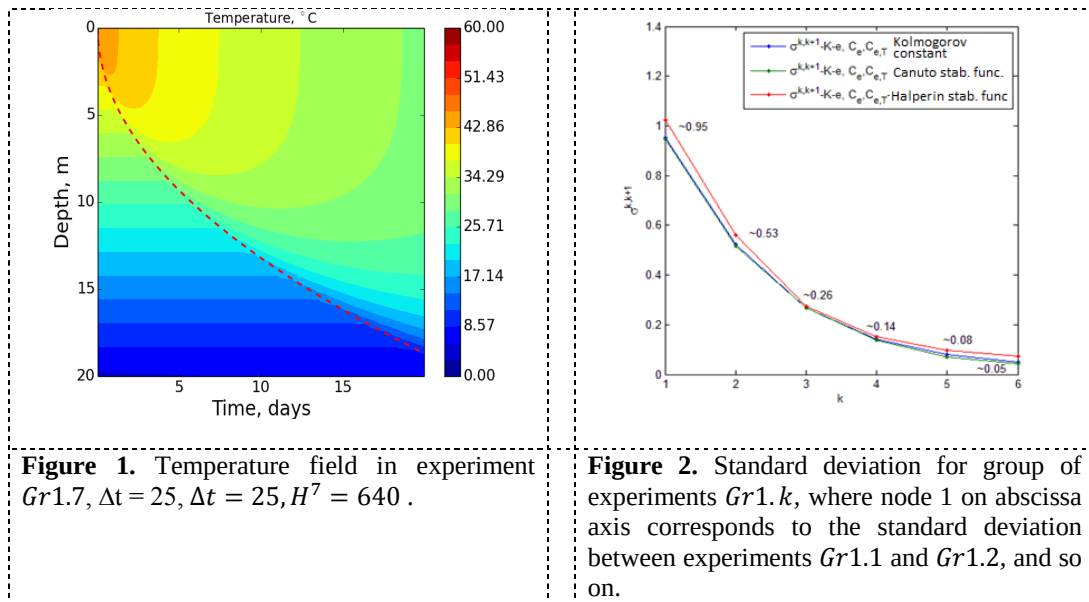
The convergence of the numerical solution was estimated using the standard deviation $\sigma^{k,k+1}$ between the temperature fields T^k and T^{k+1} (k – the experiment number) in each group of the experiments:

$$\sigma^{k,k+1} = \sqrt{\frac{1}{M*N} \sum_{i=1}^N \sum_{j=1}^M (T_{i,j}^k - T_{i,j}^{k+1})^2},$$

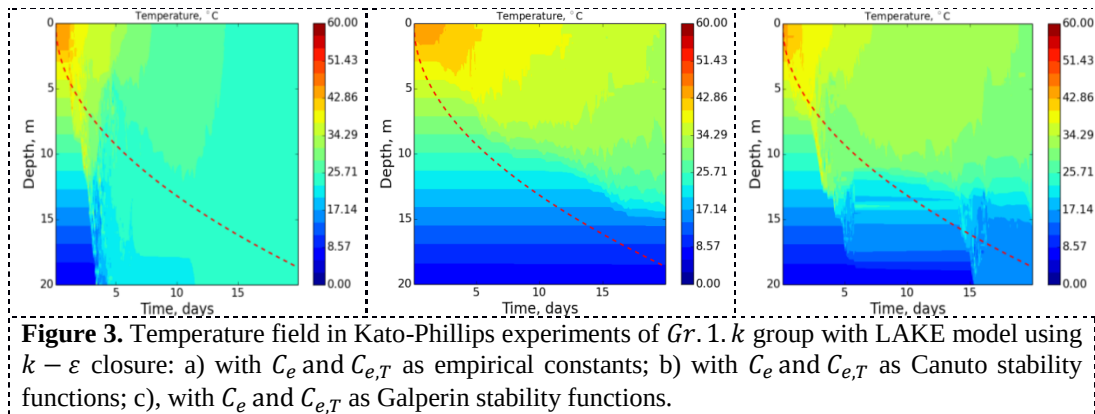
where M is the number of grid levels, and N is the number of time steps. Since the spatial and temporal resolutions differed between the experiments, to estimate the norm the results of all experiments were interpolated onto a uniform grid.

3.2. Results

The standard deviation between the results of the two experiments, Gr.1.3 and Gr.1.4, is 0.26 °C (Figure 2), and this value is close to the uncertainty of temperature measurements by standard hydrometeorological instruments. In experiments Gr.1.1, $\Delta t = 25, H^1 = 10$, there is a significant error in the mixed layer depth with respect to the analytical solution [19] for both variants of the $k-\varepsilon$ turbulence closure. One can see in Figure 1 that the mixed layer depth and the distribution of isotherms in experiment Gr.1 are almost the same and very close to the analytical solution of the mixed layer depth evolution (dashed line). Only in the case of Galperin stability functions, the mixed layer depth is less than the analytical depth by 1 m (5%). Experiments Gr.1 show that the lake model with the $k-\varepsilon$ closure calculates the mixed layer depth close to the analytical solution in experiments Gr.1.k, $k \geq 4$ ($M = 40$, with a grid spacing, $\frac{H}{M} \leq 0.5$).

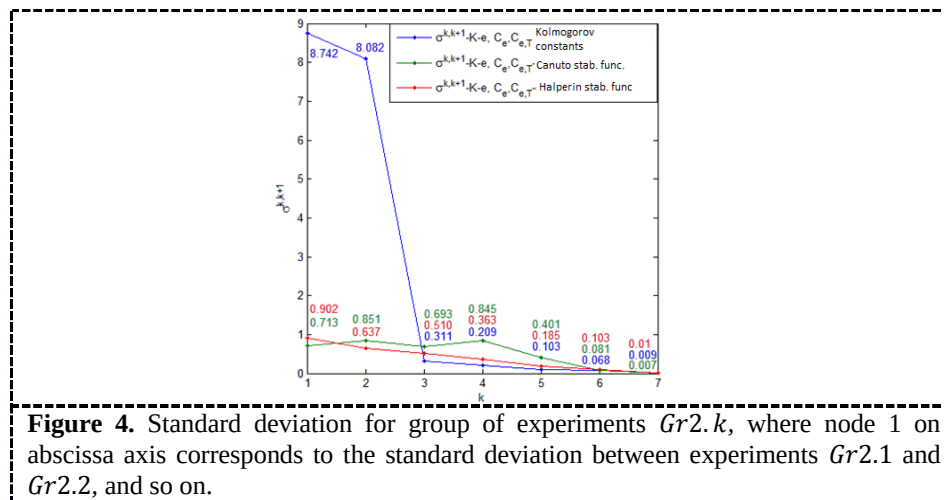


In experiments $Gr.2.1$ ($\Delta t = 3600$ s), $Gr.2.2$ ($\Delta t = 1800$ s), $Gr.2.4$ ($\Delta t = 450$ s) the numerical simulation results significantly diverge from the analytical solution (Figure 3).



In experiments $Gr.2.5$, $Gr.2.6$, $Gr.2.7$, and $Gr.2.8$, a sufficiently accurate solution for the temperature is obtained, similar to Figure 1. In this case (Figure 4), the solution with acceptable accuracy is obtained with a time step $\Delta t \leq 100$ s.

Experiments $Gr.2$ demonstrate that the model with $k - \varepsilon$ closure (with both Canuto and Galperin specifications of the Kolmogorov coefficients) provides a smooth solution only with a time step $\Delta t < 450$ s, and convergence is achieved at $\Delta t < 100$ s under stable stratification and constant wind stress.



4. Simulating a particular lake with Henderson-Sellers and k - ϵ turbulent closures

4.1. Experiment setup

The model experiment for the Kuivajärvi Lake was set with the following parameters: lake depth of 12.5 m and the meteorological data period from 1.05.2013 to 10.11.2013. The data on the atmospheric variables was provided by measurements performed by the University of Helsinki ([20], [9]).

For the LAKE model with the Henderson-Sellers parameterization, with a convective mixing scheme, two groups of numerical experiments were performed (Table 2): the first one with a varying time step Δt^k at a fixed number of vertical levels M ; and the second group with a varying number of vertical levels M^k while keeping the time step Δt constant.

Table 2. Spatial and temporal resolution in two groups of numerical experiments with Kuivajärvi Lake data.

Experiment name	Fixed param. of spatial / temporal resolution	Variable param. of spatial/ temporal resolution	Experiment Index Range
$Gr. 1.k$	$\Delta t = 25 s$	$M^k = 12; 24; 48; 96; 192$	$k = 1.5$
$Gr. 2.k$	$M = 40$	$\Delta t^k = 3600; 1800; 900; 450; 225; 100; 50s$	$k = 1.7$

4.2. Results

The experiments of group Gr.2 showed a very weak sensitivity of the LAKE model to varying the time step when using the Henderson-Sellers turbulence parameterization with a convective mixing scheme.

Experiments Gr.1 showed that the model is sensitive to the spatial resolution when $M = 12$. When reducing the spatial step the model results were changing similarly to those of Gr.2. Figures 7 and 8 show the convergence of the numerical solution with relatively coarse steps in space and time.

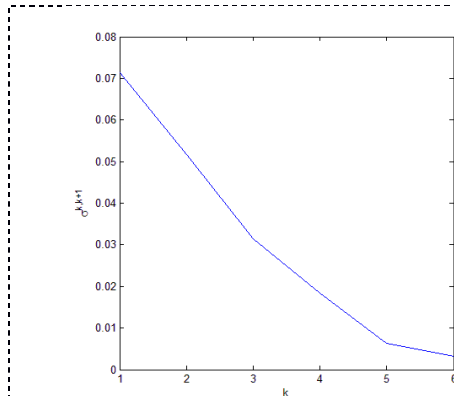


Figure 5. Standard deviation for group of experiments $Gr1.k$, where node 1 on abscissa axis corresponds to the standard deviation between experiments $Gr1.1$ and $Gr1.2$, and so on.

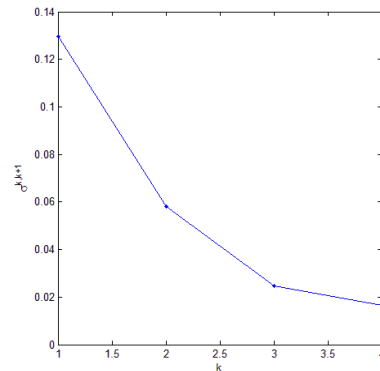


Figure 6. Standard deviation for group of experiments $Gr2.k$, where node 1 on abscissa axis corresponds to the standard deviation between experiments $Gr2.1$ and $Gr2.2$, and so on.

The experiments of group Gr.2 with the $k - \varepsilon$ turbulent closure (with different $C_e, C_{e,T}$) showed that a physically reasonable solution is attained at a time step $\Delta t \leq 450s$. For the experiments of groups Gr.2.4 and Gr.2.5 the temperature distribution is shown in Figure 7.

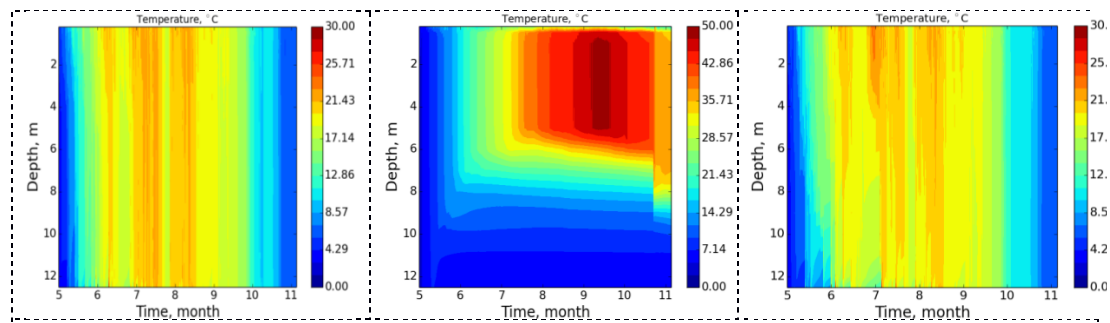


Figure 7. Temperature field of LAKE model using $k - \varepsilon$ closure in experiments of $Gr.2.4$ $\Delta t = 450s$ and $Gr.2.5$ $\Delta t = 225s$ with real atmospheric data for Kuyavarvi Lake: a) with C_e and $C_{e,T}$ as empirical constants; b) with C_e and $C_{e,T}$ as Canuto stability functions; c) with C_e and $C_{e,T}$ as Galperin stability functions.

In experiments Gr.2.6 and Gr.2.7, the temperature field was close to the measured one (Figure 8 c,d,e).

The processor wall-clock times for all experiments are given in Table 3.

Table 3. Wall-clock times of Kuivajärvi Lake simulations.

Turbulent parameterization	Δt s	M=24	M=48	M=96
Henderson-Sellers	3600s	11s	16s	18s
Henderson-Sellers	25s	192 s	247 s	349s
$k - \varepsilon$	25s	225 s	313 s	471

4.3 Comparison with measurement data

For comparison with the temporal and spatial temperature distributions obtained from measurements, model experiments were made with parameters $\Delta t = 25s, M = 48$ for the LAKE model with the $k - \varepsilon$ turbulence closure (with different variants $C_e, C_{e,T}$) and $\Delta t = 3600 s, M = 48$, with the Henderson-Sellers parameterization.

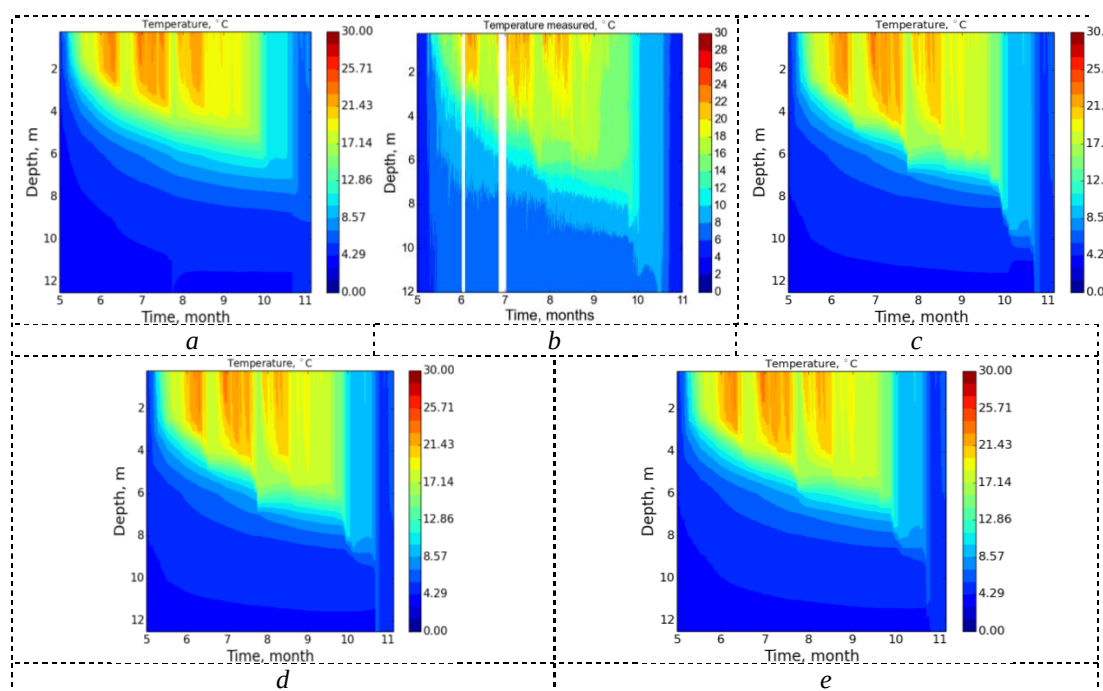


Figure 8. Temperature distribution over depth and time for Kuivajärvi Lake: a) LAKE model with Henderson-Sellers parameterization; b) measurement data [9]; c) LAKE with $k - \varepsilon$ (with Kolmogorov empirical constants) d) LAKE with $k - \varepsilon$ (with Canuto stability function); e) LAKE with $k - \varepsilon$ (with Galperin stability functions).

A comparison with the measurement data (Figure 8b) shows that the model with the Henderson-Sellers parameterization, with a convective mixing scheme (Figure 8a) qualitatively well reproduces the temperature distribution with depth, as well as the dynamics of the mixed layer, slightly lowering the depth of the latter by an average of 1 meter.

At the same time, in October and November the mixed layer depth is considerably underestimated, by 2.5–3 meters, also the model does not reproduce a jump in the mixed layer depth in August, most likely associated with a strong wind stress and surface cooling. However, these deviations are not critical for reproducing the lake surface temperature, the most important lake variable in the NWPs and ESMs.

The lake model with $k - \varepsilon$ turbulent closure (Figure 8 c,d,e) simulates sufficiently well the measured temperature distribution, the dynamics of the mixed layer depth, and the temperature “jump” in August. The mixed layer depth is reproduced in the autumn period better than when using the Henderson-Sellers parameterization. It is also worth noting that the model with $k - \varepsilon$ turbulent closure with Galperin stability functions, as well as for the Kato-Phillips experiment, underestimates the mixed layer depth and smoothes the jump characteristic of August.

5. Conclusions

The numerical experiments with the LAKE model using the $k - \varepsilon$ turbulent closure scheme with measured atmospheric forcing data have given the same results on the convergence of the solution as the Kato-Phillips experiments. The acceptable solution accuracy is achieved at $\Delta t \leq 50$ s.

The experiments with the LAKE model using the Henderson-Sellers parameterization with a convective mixing scheme have shown that acceptable solution accuracy is obtained with much more coarse steps, both in space and in time.

Our results show that the Henderson-Sellers parameterization can be used for a coefficient of turbulent thermal conductivity with $\Delta t = 3600$ s, thus reducing the computational time by 20 times compared to the calculation with $\Delta t = 25$ s.

The different versions of the $k - \varepsilon$ closure scheme reproduce equally well the dynamics of the water temperature field and the depth of the mixed layer.

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