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# Investigation and calibration of thermal and salinity layering in surface water resources using Ce-Qual-W2 model

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**Abstract:** In the discussion of water quality control, the first and most effective parameter that affects other variables and water quality parameters is the temperature situation and water temperature parameters that control many ecological and chemical processes in reservoirs. Additionally, one of the most important quality parameters studied in the quality of water resources of dams and reservoirs is the study of water quality in terms of salinity. The salinity of the reservoirs is primarily due to the rivers leading into them. The control of error in the reservoirs is always considered because the outlet water of the reservoirs, depending on the type of consumption, should always be standard in terms of salinity. Therefore, in this study, using the available statistics, the Ce-Qual-W2 two-dimensional model was used to simulate the heat and salinity layering of the Latyan Dam reservoir. The results showed that with warming and shifting from spring to late summer, the slope of temperature changes at depth increases and thermal layering intensifies, and a severe temperature difference occurs at depth. The results of sensitivity analysis also showed that by decreasing the wind shear coefficient (*WSC*), the reservoir water temperature increases, so that by increasing or decreasing the value of this coefficient by 0.4, the average water temperature by 0.56°C changes inversely, and the results also show that by increasing or decreasing the value of the shade coefficient by 0.85, the average water temperature changes by about 7.62°C, directly.

**Keywords:** Ce-Qual-W2 model, salinity, surface water, thermal layering, water quality modelling, water resources

## INTRODUCTION

Ensuring a supply of drinkable water is one of the most fundamental issues for human life. The primary sources of fresh water, although renewable, are limited in quantity. As has been the custom for a long time, the need to store water through the construction of dams and reservoirs is a suitable solution for water supply for agriculture, industry, drinking, flood control, hydropower generation, etc. [Molajou *et al.* 2021; Nourani *et al.* 2020]. These amounts can be made available to users when large amounts of water are stored and large reservoirs are available. The quality of the water stored in these reservoirs and the water made available to others is an issue that has always been under scrutiny to determine if it is suitable for various purposes. Therefore, using simulation models, the ability to predict and evaluate water quality in reservoirs in the management of water resources is a very important issue that leads to work progress [Azadi *et al.* 2019; Hua, Zhang 2017; Melo *et al.* 2019].

River water flow is affected by processes such as aeration, cellular respiration, and mixing; it has a uniform quality. Therefore, water quality will change when the construction of a dam is stopped. The most important changes that may occur are temperature layering and consequently layering of other qualitative components in the dam reservoir. In addition to temperature, the concentration of soluble solids, which is an indicator of salinity in a reservoir and running water, is an important factor affecting the reservoir's layering, and it is necessary to study [WU *et al.* 2018; ZHI *et al.* 2021].

The main difference between lakes and reservoirs and rivers is speed. The nature of river flow causes complete mixing in depth and width. This contrasts with the gentle flow in reservoirs and lakes tends to layer and slow the transfer. In modelling the water quality of lakes and reservoirs, the thermal regime is important from two perspectives. First, the temperature directly affects the rate of chemical reactions, and second, heat balance has a significant effect on mixing in freshwater systems [AFSHAR *et al.* 2021; DOÑA *et al.* 2014; HAMILTON, SCHLADOW 1997; SCHLADOW, HAMILTON 1997; WANG *et al.* 2019].

The thermal regime is mainly the result of the interaction of two processes of heat energy transfer from the lake surface and the effect of gravity on the density difference [SKOWRON, PIASECKI 2016]. Depending on the season, heat exchange in the joint season of lake surface and air leads to an increase or decrease in water surface temperature due to factors such as solar radiation energy, air temperature, relative humidity, wind speed, and sky cloud percentage. Wind on the lake's surface leads to mixing the surface part of the water and heat transfer and downward movement. In opposition to mixing, there is a buoyancy force that prevents further mixing. This force is created by the difference in density at different temperatures and causes the denser part of the water to be at the bottom [CAISSIE 2006; CHENG *et al.* 2020; WANG *et al.* 2012].

The pattern of stratification and the number of complete mixes in lakes and reservoirs depends on its geographical and meteorological characteristics. The number and frequency of mixing have a direct effect on water quality. Given that stratification significantly impacts the water quality of lakes and reservoirs, it is important to predict the stratification potential. The stratification potential of lakes and reservoirs is a function of heat exchange, lake depth, reservoir shape, water flow, and wind speed. It should be noted that there are different methods for estimating stratification potential that can be selected depending on the nature of the work and the importance of the issue.

Although the basic assumption of many simple models for lakes and reservoirs is complete reservoir mixing, this assumption is not generally true. Changes in water density with temperature cause lakes and reservoirs to usually be layered. Layering means forming layers of fluid masses suspended due to differences in density, temperature, or materials. In deep reservoirs, the temperature difference between the top and bottom layers can reach more than 15°C. In most reservoirs and lakes, stratification is the result of the thermal balance between inhibited water and other inlets to the reservoir. Inlet heat includes atmospheric and solar radiation, heat exchange between water and the atmosphere, and heat from inlet currents to the reservoir. Water heat can be lost due to surface radiation, evaporation, and heat transfer [HENRY 1993]. Most heating and cooling processes occur in a relatively thin surface layer. Therefore, if vertical mixing is not sufficient to equalise the surface gradient, thermal layering is formed. In this regard, reservoirs are divided into three categories: unlayered, weakly layered, and severely layered. In reservoirs with vertical mixing, the temperature and density at depth are uniformed in winter and summer. Poorly layered reservoirs are characterised by isothermal lines tilted along the horizontal axis. Deep reservoirs with intense stratification are characterised by horizontal temperature lines along the reservoir and have seasonal stratification of temperature or density. At the time of stratification, the following three distinct layers are formed in the reservoir [LITVINOV, ZAKONNOVA 2012; YANG *et al.* 2020].

1. **Top layer** – the higher the area, the warmer and the lower the density. This layer is thin, warm, and generally a relatively fresh layer with a temperature that is almost constant and high. The thickness of the surface varies from lake to lake and from month to month. This layer may be only about one meter in small lakes, while in large lakes, it may exceed 20 m.
2. **Sublayer two or bottom layer –** the lower the area, the colder and denser. This cold layer has more salinity and a lower thermal gradient at the bottom of the reservoir.
3. **Interlayer or transition layer** – the area between the layer and the substrate. The temperature changes drastically between the layer profiles at depth, which limits the vertical transfer of heat and momentum. Hence, it causes the separation of hydraulic, temperature, and ecological characteristics in the two layers of the lake. The depth of this layer varies due to wind and mixing and heat exchange on the lake surface. In lakes located in the middle latitude, the useful depth between the layers is between 5 and 15 m, and the temperature difference between them is between 10 and 20°C. The interlayer region is also called mesolimnion 3 and metallimnion 4.

As mentioned before, in addition to temperature, the concentration of soluble solids, which is an indicator of salinity in reservoirs and water bodies, is an important factor that affects the stratification of the reservoir, and it is necessary to study. It should be noted that total soluble solids (*TDS*) vary with salinity. Water salinization occurs due to the presence of some anions (chlorine and sulphate) and cations (sodium and potassium). However, since the most important part of *TDS* is salinity, *TDS* is used as an indicator to estimate the salinity of water bodies. The main factors influencing the salinization of water bodies are atmospheric factors, geological factors, and hydrological factors. Increasing salinity increases the density of water; it is also one of the factors causing the stratification of reservoirs. It should be noted that in this study, salinity is the same as *TDS*.

## MATERIALS AND METHODS

### CE-QUAL-W2 MODEL

Qualitative reservoir simulation is one of the available solutions to know the current status of a reservoir and predict future conditions. Water quality models can be classified according to the dimension (one-dimensional, two-dimensional, three-dimensional), the pollutants they simulate (phosphorus, nitrate, or other toxic substances), and the system in which they are applied (lake or river).

With the advancement of knowledge and technology, many phenomena are simulated by mathematical models and computer programs according to the governing differential equations and the observations and results of physical models. It used three-dimensional hydrodynamics with equations of transfer and physical and chemical reactions. To accurately predict thermal layering and water quality, the use of a two-dimensional model-averaged in width is inevitable. In two-dimensional modelling, a suitable and accurate method is simultaneous modelling of flow hydrodynamics and qualitative parameters [Debele *et al.* 2008; Khodabandeh *et al.* 2021].

Fluid motion is modelled using mass, momentum, and energy survival equations. In many turbulent flows, the Reynolds equations, which model the turbulent three-dimensional motion of a fluid in a mediated time, can be used with great accuracy. If the changes in width are insignificant compared to the changes in length and height, the equations in width can be integrated, and the averaged equations in Reynolds width can be obtained. These equations are the basis of many models averaged across the quality of dam reservoirs [Ostfeld, Salomons 2005].

The CE-QUAL-W2 model is a two-dimensional (horizontal and vertical) model for modelling hydrodynamics and water quality that can model structures such as deep rivers, dam reservoirs, and lakes. This model was developed in 1995 by the U.S. Army Corps of Engineers, Waterways Experimental Station (WES), which is based on solving two-dimensional hydrodynamic equations (unsteady) and advection dispersion. This software can predict the behaviour of aquatic ecosystems, including dam reservoirs, by mathematical simulation. If the minimum amount of necessary information is available, the results of this model will be acceptable. Some of the capabilities of this simulator model for mathematical simulation are as follows [Deliman, Gerald 2002]:

1) changes in water level, water velocity, and temperature are dynamically predictable;
2) various factors of determining water quality can be simulated or removed from the simulation by the user's choice;
3) this model can be used in various water systems such as rivers, dam reservoirs, lakes, estuaries, and combinations of those mentioned above;
4) by dividing the water body and determining the segment and layer, it can be used in various shapes of water environments with different dimensions and depths;
5) the model has enough flexibility to select the type and number of computational results to be obtained;
6) the results of model calculations can be obtained from computer screen, print and plot. The user can also specify the time period and the number of required results during the simulation period during the simulation.

## CASE STUDY

In this study, the reservoir of Latyan Dam has been studied. The catchment area of Latyan Dam with an area of 690 km$^2$ is located in the west of Damavand city and northeast of Greater Tehran and within the city of Shemiranat (35.7901°N, 51.6785°E). This basin is a mountainous basin, so that about 90% of it consists of mountains and hills. Its highest point is 4000 m a.s.l., and its lowest point is Latyan Dam reservoir, with an altitude of about 1600 m a.s.l. [Mohseni-Bandpei *et al.* 2018].

The reservoir's geometric and depth information has been extracted from topographic maps with a scale of 7500:1. In order to introduce the dam reservoir to the model, the dam reservoir was transformed into two water bodies that include the entrance of two separate rivers. The inflow water bodies from each of the rivers were divided into 15 sections (or steps) along the reservoir. Also, each of these water bodies was deeply divided into 48 layers (Figs. 1, 2).

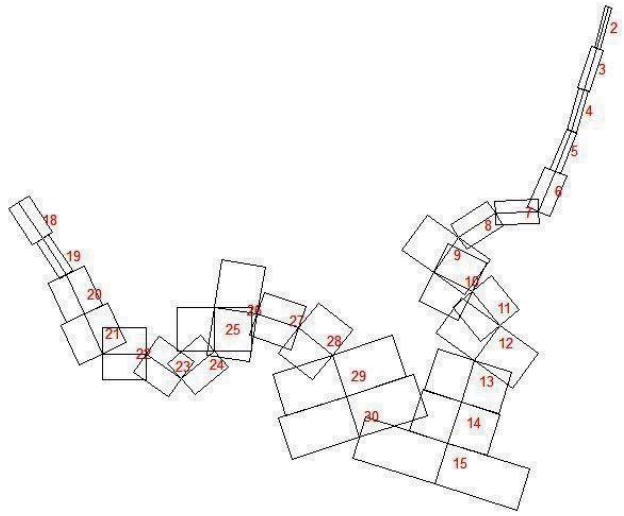

**Fig. 1.** The geometric shape of the reservoir, along; source: own elaboration

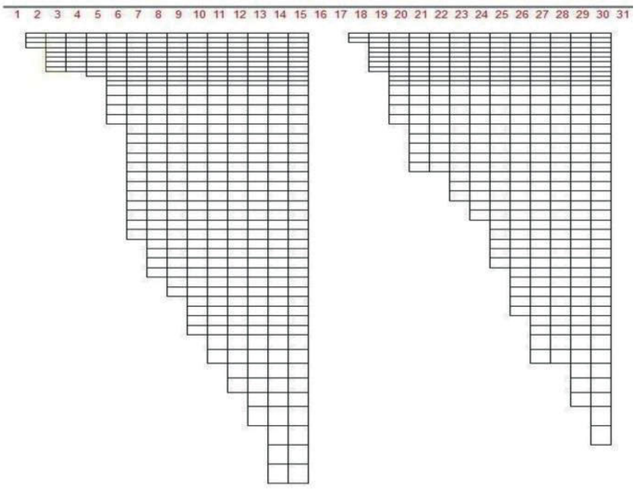


**Fig. 2.** The geometric shape of the reservoir's depth; source: own elaboration

## METEOROLOGICAL FILE

Meteorological data, including wind speed and direction, air temperature, dew point temperature, and cloud cover, were extracted from the nearest meteorological station and based on daily data whose statistical characteristics (including average, minimum value, maximum value, and standard deviation) were reported in Table 1.

**Table 1.** Statistical specifications for daily observational data

| Parameter | Average | Minimum value | Maximum value | Standard deviation |
|---|---|---|---|---|
| Air temperature (°C) | 15.107 | –13 | 41 | 11.243 |
| Dew point temperature (°C) | –0.957 | –26 | 17 | 5.325 |
| Wind speed (m·s$^{-1}$) | 2.234 | 0 | 9 | 2.015 |

Source: own elaboration.

### CONDITIONS FILE

The initial conditions file contains information about the quality of the reservoir on the first day of the simulation. The first day of the simulation is marked as day 601. It should be noted that the last day is 1097.

The upstream boundary conditions are introduced into the model by the inlet flow to the reservoir and the inlet water temperature. The downstream conditions are introduced to the model by the outlet flow from the reservoir.

## RESULTS AND DISCUSSION

Reservoir water quality depends on various factors such as catchment, the climate of the region, especially the geometry and characteristics, and internal processes of the reservoir. In addition, water quality is affected by the type and location of the reservoir and how to use the reservoir control capabilities. To understand how to develop water quality conditions, the interaction of all dynamic phenomena in the reservoir must be studied. Figure 3 shows diagrams of water level, temperature, and salinity at current conditions relative to time (days).

Then, to investigate the occurrence or non-occurrence of thermal layering in different months, a graph of temperature changes in depth was drawn for the whole study period on a monthly basis (see Fig. 4).

According to the diagrams drawn in Figure 5, in the first month of the simulation, which is marked in the diagram with the number 601 (from mid-August to mid-September), when the weather is almost cold, no thermal layering is created [Khodabandeh *et al.* 2021]. Then, with decreasing temperature, which can be related to late autumn and winter, the height of the surface is increased until the temperature is fixed at depth and the state of the reservoir is in full mixing. Finally, with the warming of the air, which is related to the change of seasons to spring and early summer, thermal layering has occurred. With warming and shifting from spring to late summer, the slope of the changes increases and the thermal layering intensifies, and a sharp temperature difference in depth is observed. Figure 5 shows a graph of in-depth salinity changes (*TDS*) for the entire study period on a monthly basis (30 days).

As shown in these diagrams in Figure 5, during the layering period (early spring to late summer) with increasing depth, the concentration of *TDS* increases, and during the mixing period, the concentration of this parameter at different depths of the reservoir is approximately constant.

In most quantitative and qualitative research, finding the most important influential factors has always been one of the concerns of researchers. The reason is the more complex relationships between variables and phenomena under study. In this regard, the dependent variable is not only affected by an independent variable, but there are many known and unknown variables that affect the dependent variable. A set of other variables may influence the variables themselves. Therefore, identifying which variable can have a more significant impact on the dependent variable becomes challenging, and a concept called sensitivity analysis is introduced. In other words, sensitivity analysis is the study of the effect of output variables on the input variables of a statistical model. In other words, it is a way to

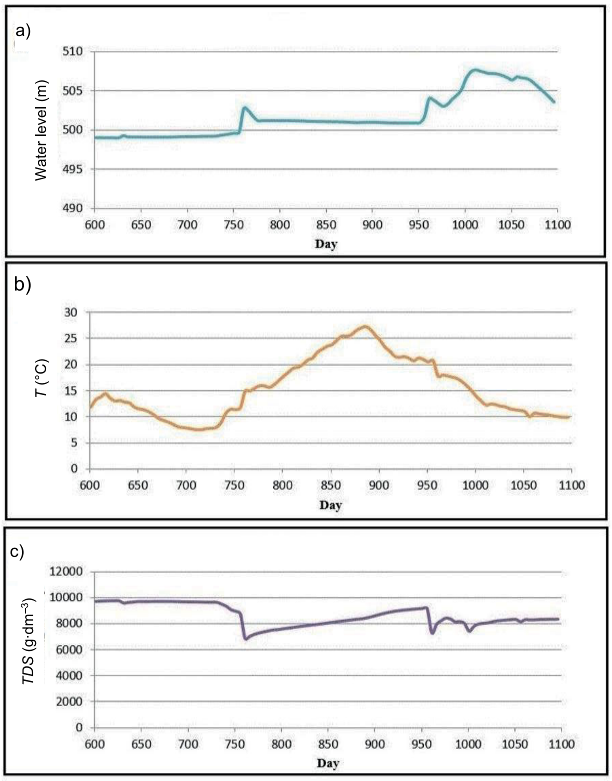


**Fig. 3.** Diagrams of: a) water level, b) temperature, c) salinity; source: own study

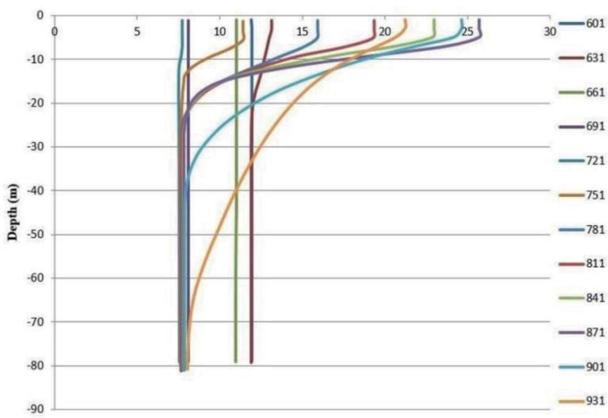


**Fig. 4.** A diagram of temperature changes in depth; source: own study

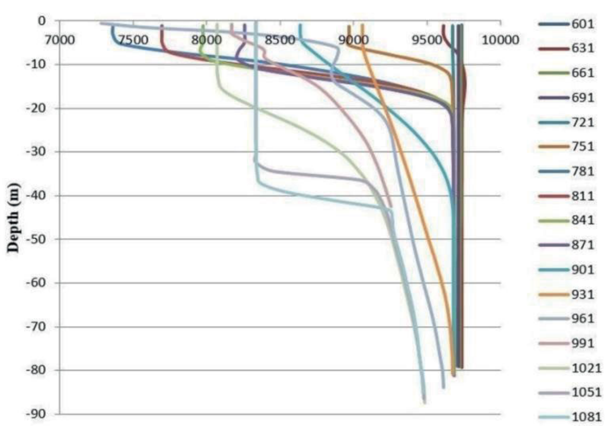


**Fig. 5.** A diagram of total dissolved solids (*TDS*) changes in depth; source: own study

change the inputs of a statistical model in an organised (systematic) way that can predict the effects of these changes on the output of the model.

By changing one parameter and keeping the other parameters constant, the effect of that parameter on temperature and salinity can be investigated. The parameters which are evaluated and analysed can include natural and human factors. Wind coefficient (*WSC*) and shadow coefficient (shade) are two parameters that have been evaluated in this study, and sensitivity analysis has been performed on them. Figures 6 and 7 show temperature and salinity diagrams for three different values of coefficient, respectively. They show wind cover (*WSC* = 0.5; *WSC* = 0.9; and *WSC* = 1.0) as well as three different values of the shadow coefficient (shade = 0, shade = 0.85 and shade = 1).

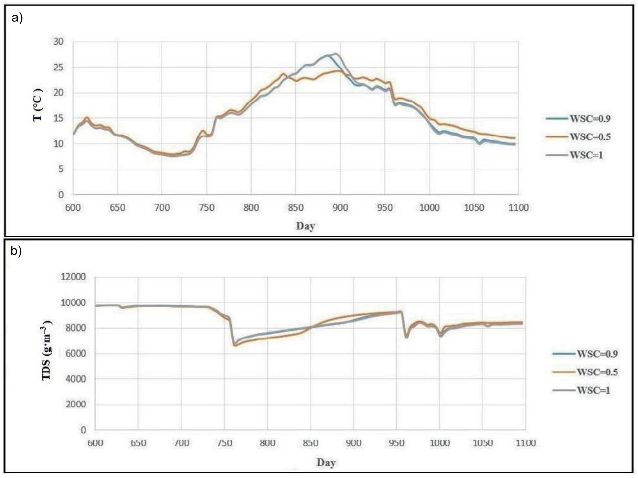


**Fig. 6.** Changes of: a) temperature (*T*), b) total dissolved solids (*TDS*) for different values of wind shear coefficient (*WSC*); source: own study

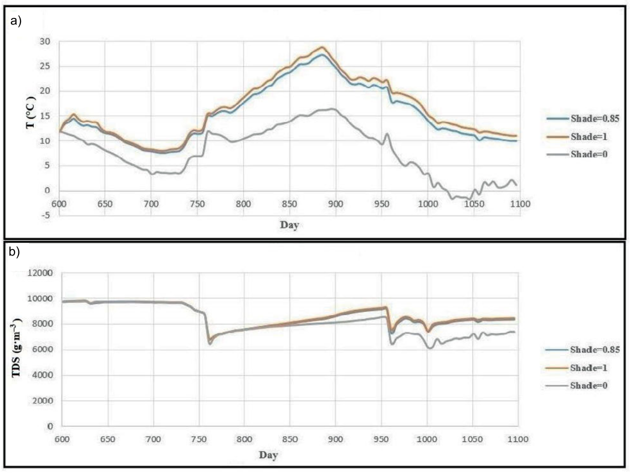


**Fig. 7.** Changes of: a) temperature (*T*), b) total dissolved solids (*TDS*) for different shade values; source: own study

According to the text of the CE-QUAL-W2 software user guide, the *WSC* is one of the most important parameters that can affect the temperature during the calibration process and must be adjusted at the very beginning. This coefficient is proposed for mountainous areas as well as rural areas with dense texture, a number between 0.5 to 0.9, and for open areas is 1.0. This coefficient can be even more than 1.0 in rare cases. In this study, three different values of *WSC* (*WSC* = 0.5; *WSC* = 0.9; and *WSC* = 1.0) were evaluated. As shown in Figure 7, by decreasing this coefficient, the water temperature of the reservoir increases, so that by increasing or decreasing the value of this coefficient by 0.4 (comparing the state of *WSC* = 0.9 with *WSC* = 0.5), the average water temperature changes inversely by about 0.56°C.

Shade fraction is a value between zero and one; the number one means no shadow, and the number zero means full shadow, which means that sunlight is reduced by 100%. Reservoirs are usually made in hollow areas, and the probability of shadowing on them is a number between zero and one. In other words, the higher this coefficient and the closer to one, the probability of shadowing on the reservoir is low. The closer the number is to zero, the larger the area of the reservoir is in shade. In other words, the higher this coefficient, the lower the probability of shadow falling on the reservoir, and the smaller this number means that most of the reservoir is in the shade. In this study, three different values of the shade coefficient (shade = 0, shade = 0.85, and shade = 1.0) were evaluated, and as shown in Figure 7, the reservoir water temperature decreases by decreasing this coefficient.

The selected scenarios can be natural scenarios or exploitation scenarios. The selected scenarios of natural factors are based on climate change. For example, the weather may get warmer in one year, or the wind may increase on average per year [Wang *et al.* 2012]. Operational scenarios also depend on the management and executive policies. In this study, a realistic scenario is defined, and its effect on the temperature and salinity of the reservoir is discussed.

In this scenario, it is assumed that the air temperature ($T_{\mathrm{air}}$) will be 20% warmer or colder than the current conditions. In other words, the air temperature data has once decreased by 20% ($0.8T_{\mathrm{air}}$) and once increased by 20% ($1.2T_{\mathrm{air}}$) and compared with the conditions of existence ($T_{\mathrm{air}}$). Figure 8 shows the effect of this increase and decrease of air temperature on the level of water level, temperature, and salinity compared to existing conditions.

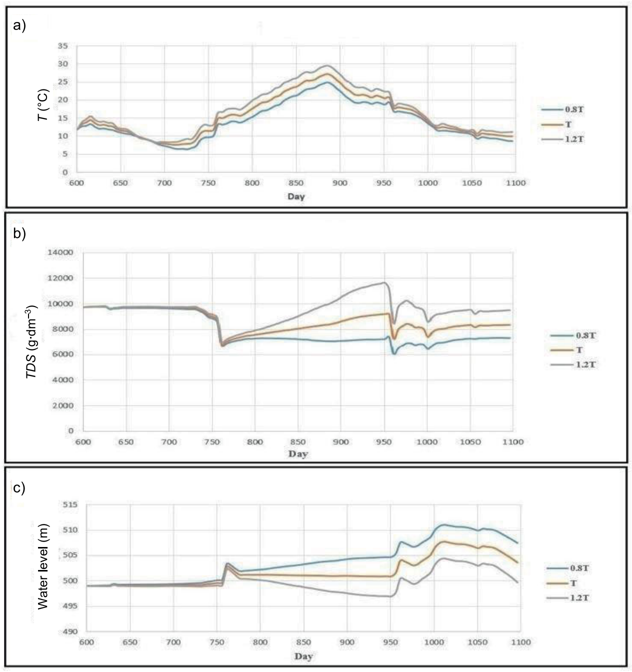


**Fig. 8.** A diagram of the effect of 20% increase and decrease of air temperature on: a) temperature, b) salinity, c) water level; source: own study

As shown in the diagrams in Figure 8, with increasing $T_{air}$, the water temperature and the amount of salinity have increased. However, the water level has decreased, and vice versa. Therefore, the water level and, as a result, the volume of water in the reservoir decreases. This factor causes the salinity concentration to increase so that with a 20% increase in air temperature, the reservoir temperature and the average salinity concentration are 1.32°C, respectively and 736.448 g·m$^{-3}$ increased. As a result, the average level of the reservoir decreased by 2.0286 m.

## CONCLUSIONS

The occurrence of processes such as thermal layering in reservoirs causes a severe decline in water quality and failure to provide the desired level for various uses and endangers the aquatic life of the downstream ecosystem. In addition to temperature, total dissolved solids (*TDS*), which is an indicator of salinity in reservoirs and water bodies, is an important factor affecting the reservoir's layering, and it is necessary to study. Therefore, this study aimed to simulate temperature and salinity in the surface reservoir of Latian Dam for one year using the CE-QUAL-W2 model.

The results showed that with warming and shifting from spring to late summer, the slope of temperature changes at depth increases and thermal layering intensifies, and a severe temperature difference at depth occurs. The sensitivity analysis results also showed that by decreasing the wind speed coefficient (*WSC*), the reservoir water temperature increases, so that by increasing or decreasing the value of this coefficient by 0.4, the average water temperature by 0.56°C changes inversely. The results also showed that by increasing or decreasing the value of the shade coefficient by 0.85, the average water temperature changes by about 7.62°C directly. With increasing this coefficient, the amount of salinity also increases relatively.

Also, the results related to the definition of natural scenario showed that with increasing air temperature, water temperature and salinity increase and the water level decreases, and vice versa, so that with a 20% increase in air temperature, reservoir temperature and also, the average salinity concentration increased by 1.32°C and 736.448 g·m$^{-3}$, respectively, and the reservoir level decreased by an average of 2.0286 m.

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