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MODELING SURFACE WATER QUALITY AND NUTRIENT CORRELATION
WITH SEDIMENT OXYGEN DEMAND AT DAM WATER RESERVOIR

THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
ATILIM UNIVERSITY

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DOCTOR OF PHILOSOPHY THESIS
IN
THE DEPARTMENT OF MODELING AND DESIGN OF ENGINEERING
SYSTEMS (MAIN FIELD OF STUDY: CIVIL ENGINEERING)

ATILIM UNIVERSITY 2022

June 2022

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A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
ATILIM UNIVERSITY

BY

NOOR N.ABDULQADER

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF DOCTOR OF PHILOSOPHY
IN
THE DEPARTMENT OF MODELING AND DESIGN OF ENGINEERING
SYSTEMS (MAIN FIELD OF STUDY: CIVIL ENGINEERING)

June 2022

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ABSTRACT

Modeling Surface Water Quality and Nutrient Correlation with Sediment Oxygen Demand at Dam Water Reservoir

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May 2022, 87 pages

The work presented here is a model approach based on WASP8 (Water analysis simulation program) a water quality model simulated to represent contaminants at the surface and bottom sediments of the Kurtboğazı dam reservoir in Ankara. Investigated water quality output variables were temperature, nitrate, total phosphorus, total Kjeldahl, dissolved oxygen, Chlorophyll a, and ammonium. To ensure that the model represents the actual case at the reservoir, the results from our simulation model were calibrated using actual data from the Kurtboğazı dam site, and the calibration utilizes statistical techniques. The novelty of this research is the development of a quality model to predict the reactions of state variables that are occurring at the water body and how they interact with each other and their influence on the overall quality status of the Kurtboğazı reservoir, as well as the crucial factors influencing the depletion of oxygen at the water column. The accuracy of the model was checked using statistical techniques in the form of coefficient of determination and relative error which produced excellent ranges of results indicating that our simulated model was able to represent the features at the reservoir site. The Kurtboğazı dam reservoir had been affected by the negative impact arising from dissolved oxygen depletion in the hypolimnetic layer during stratification periods. However, the processes of oxygen consumption at the sediment-water interface are still difficult to grasp conceptually and are mainly linked to sediment oxygen depletion and the phenomena of sediment oxygen demand SOD. The work here presents a simulation model that can be utilized as a helpful tool by any person working in the sector of water management, to estimate and predict the parameters influencing the anoxic condition and benthic flux.

Keywords: Water quality; Dam reservoir; Nutrients; SOD; WASP8 model.

ÖZ

BARAJ REZERVUARLARINDA SEDİMENT OKSİJEN İHTİYACI İLE SU KALİTESİ VE BESİN MADDE İLİŞKİSİNİN MODELLENMESİ

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Mayıs 2022, 87 Sayfa

Burada sunulan çalışma, Ankara'daki Kurtboğazı baraj rezervuarının yüzey ve dip çökelilerindeki kirleticileri temsil etmek üzere simüle edilen bir su kalitesi modeli olan WASP8'e (Su analizi simülasyon programı) dayalı bir model yaklaşımıdır. Çalışmada yeralan su kalitesi değişkenleri şunlardır: sıcaklık, nitrat, toplam fosfor, toplam Kjeldahl, çözünmüş oksijen, Klorofil a ve amonyum. Rezervuardaki gerçek durumu temsil etmesini sağlamak için simülasyon modelimizin sonuçları Kurtboğazı baraj sahasından alınan gerçek veriler kullanılarak kalibre edilmiş ve istatistiksel verilerden yararlanılmıştır. Bu çalışmada özgün olarak, su kütlesinde meydana gelen durum değişkenlerinin tepkilerini, birbirleriyle nasıl etkileşime girdiklerini ve bunların Kurtboğazı rezervuarının genel kalite durumu üzerindeki etkilerini tahmin etmek için bir kalite modelinin geliştirilmesi araştırılmıştır. Modelin doğruluğu, simüle edilmiş modelimizin rezervuar alanındaki özellikleri temsil edebildiğini gösteren mükemmel sonuç aralıkları üreten belirleme katsayısı ve bağıl hata biçimindeki istatistik teknikleri kullanılarak kontrol edilmiştir. Kurtboğazı baraj rezervuarı, tabakalaşma dönemlerinde hipolimnetik tabakada çözülmüş oksijen tükenmesi gibi olumsuz etkilerden etkilenmiştir. Bununla birlikte, tortu-su arayüzündeki oksijen tüketimi süreçlerini kavramak hala zordur. Temel olarak, tortu oksijen tükenmesi ve tortu oksijen talebi SOD ile bağlantılıdır. Bu nedenle, bu model, su yöneticileri için anoksik durumu ve bentik akıyı etkileyen parametrelerin tahmini için faydalı bir araç olarak hizmet edebilir.

Anahtar Kelimeler: Su kalitesi, Baraj Rezervuarı, Besin, SOD, WASP8 model

ACKNOWLEDGMENTS

I would like to express my profound gratitude and appreciation to my supervisor Assist. Prof. Dr. Enver Güler (Department of Chemical Engineering/Atilim University/Ankara) has always provided me with resources and this work was completed under his guidance and support.

I'm forever indebted to Professor Dr. Belgin Sultan İşgör (Department of Applied Chemistry/Atilim University/Ankara), for her helpful guidance, support, and precious suggestions throughout this study.

Furthermore, I thank my co-supervisor Assoc. Prof. Dr. Aslı Numanoğlu Genç (Department of Civil Engineering/TED University/Ankara) gave me freedom in my vision to pursue my research.

Special thanks to the staff at ASKI (Directorate General of Ankara Water and Sewerage Administration) in Ankara for their cooperation and support in providing necessary data for the Kurtboğazi dam reservoir.

Finally, special thanks to my family and my colleagues for their support and encouragement, with endless patience and sincerity throughout this period.

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CHAPTER 1

INTRODUCTION

There is an increasing problem of rapid population growth, which results in many countries either suffering water shortage or will eventually face this issue in the future, and due to the ever-growing anthropogenic activities which have exacerbated water resources depletion on a global scale. In addition to anthropogenic activities, climate change exerts extra pressure on water availability in many regions around the world. Eventually, the human activities from agriculture, wastewater removal, growing industries, etc., will only contribute to the problems of surface water pollution [1, 2].

Ankara is considered to be the largest and most heavily populated city located at the heart of the central Anatolia region, in Turkey the annual precipitation of Ankara is variable and to avoid potential problems, Dam (Çubuk-II, Bayındır, Kurtboğazi, Çamlıdere, Eğrekkaya, and Akyar) are built. These dams avoid water shortage; flooding; provide irrigation generating power and recreational areas [3], these reservoirs obtain their names from the dam constructed at the location: also, undoubtedly water quality in these reservoirs is affected by the inflow of water, climate changes and total resident time at reservoir [4].

An increasing number of environmental engineers and managers are becoming aware of the growing dilemma regarding population growth and resources scarcity, they managed to resolve this issue by using alternative prevention systems to minimize water contamination and pollution through the use of modeling and simulation which eventually was found to be by far much more practical more efficient than the conventional water quality strategies that require large capital investment [5]. The fundamental function of a simulation model is to depict all the temporal and spatial activities of the natural environment, however, these activities are influenced by the chemical and physical reactions that take place in the system. The important notion to consider is the influence and external factors that integrate in to the dynamic of that system.

Water Quality Analysis Simulation Program WASP is known to be a versatile dynamic segment-based software package program that can be applied to different water sources such as lakes, reservoirs, rivers, and their associated aquatic life systems, the program simulates the effects caused by human activities of the consequences of natural phenomena impacting the water body. Figure 1.1, is an outline of the system sequence for the model. The WASP is a simulation program used in many systems: for example, estimation of pollution load for the Taipu River [6]; total maximum daily load analysis TMDL for nutrients in the Neuse River Estuary, North Carolina [7]; phytoplankton in St. Louis Bay, Mississippi [8]; impacts of climate change on water quality of Chungju Lake-South Korea [9]; dissolved oxygen in the Danshui and Chungkang Rivers, Taiwan [10]; dissolved oxygen depletion in diverted floodwaters of the Elbe River, Germany [11]; eutrophication control in the Keban Dam Reservoir, Turkey [12].

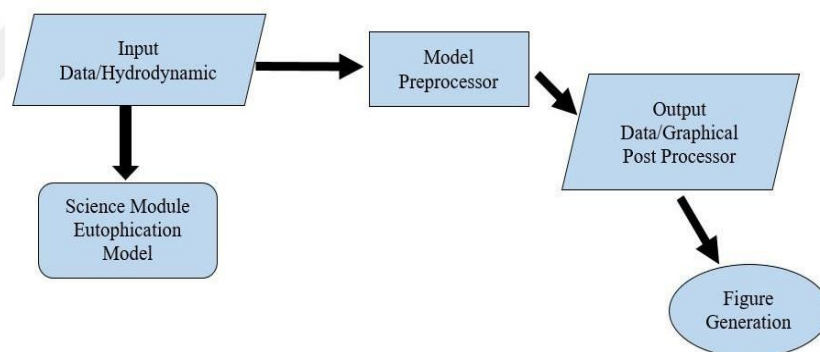


Figure 1.1 Model framework

Part of a thorough and accurate water management system is the understanding of the dissolved oxygen level in the water body. DO is considered a dominant factor to measure a healthy ecosystem. However, numerous important elements contribute to DO levels in surface waters, such as reaeration from the atmosphere; however, inflowing waters that convey organic material into a reservoir have a counter-back impact and this stuff settle in the sediments along the benthos zone [13]. However

the remains of dead plants that undergo decomposition will consume oxygen and go through biochemical oxygen demand (BOD), and on the sediments, known as sediment oxygen demand (SOD) [14]. Any organic material when undergoing the process of degradation in the sediment will require oxygen and that eventually causes the depletion of O₂, however, the decrease of oxygen will reflect on the surface water quality in what is known as sediment oxygen demand SOD there, some numerous factors and parameters influence sediment oxygen demand: are water temperature, type of sediment, depth of water body, the velocity of water, and the total surface area. SOD governs and influences reactions in sediment and the water column, one of these harmful phenomena is eutrophication or the harmful algal blooms which eventually cause oxygen depletion or hypoxia [15].

1.1 Literature Review

Water quality management is an important component of fully integrated water resource management. This feature may arise due to the growing customers' demand for potable water therefore, authorities in the water sector are obliged to make all the necessary efforts to achieve that goal for customers, it has been observed that significant efforts are being accomplished in that field. An important notion that must be understood is that the water quality in nature has an impact on the status of ecosystems, as well as on humans consuming these waters. Over the years an increasing number of models are simulated and developed to mimic field status to predict the possibility of pollution and contaminations, thus, making the necessary decisions for their removal from the ecosystem.

1.1.1 Cases of the spatial distribution and integrated

There are plentiful research and case studies revolved around the application of the WASP such as in the case of the Duriangkang dam which was focused on modeling the water quality parameters including dissolved oxygen, total phosphorus, and biochemical oxygen demand, and conducting the calibration it was evident that the model simulated results that were in excellent fit with field data from the actual site [16]. In a research study carried out at Sulejów Reservoir, the

WASP model was used to simulate the water quality, when analyzing the model results it helped the managers to conclude that when the phosphorus and nitrogen quantity was cut down by 50% the reservoir can sustain an acceptable quality of water [17]. As for the Shenandoah River basin the WASP simulation program guided the planners to fully understand the complexity of nutrients, dissolved oxygen DO, and chlorophyll-a dynamics at the basin and how different parameters interact with external influent to reflect the overall water quality [18]. In North Carolina at Cape Fear River, the water body was examined using WASP's advanced toxicant module which included examining the nanoparticles in the water column and modeling light intensity and photoreactions [19]. In the Anacostia River's tidal part the WASP toxicant model successfully simulated toxic metals and was able to determine the quantities of these concentrations at different times of the year in the water column [20]. A key factor for the effectiveness of the WASP simulation model is its capability to guide the management strategy to select the best strategic plan to control contamination of the water body [21]. The seasonal changes impacted the ecosystem at Ravi River in Punjab, Pakistan, with the assistance of the WASP modeling program the managers were able to locate the source of pollution along the river and put forward a possible strategy plan to eliminate and minimize their impact [22].

1.1.2 Contribution of sediment oxygen demand SOD on water quality

The fundamental parameter affecting the health status of an ecosystem is oxygen level. Therefore factors causing depletion of the oxygen are considered crucial elements. Sediment oxygen demand describes the decrease of oxygen level or the oxygen decrease rate caused by the oxidation of organic matter and also the respiration of plants at benthic [23]. According to experimental work determined by the Environmental Protection Agency research laboratory [24], the velocity of water influences the sediment oxygen demand, other factors include the dissolved oxygen DO transport across the water boundary layer. The explanation for this phenomenon is through microbial action which increases the rate of transit of DO into the sediments. When the water body has a low-velocity rate and high level of organic matter in the benthic layer this will cause a low dissolved level of oxygen in the

water column, and this phenomenon occurs annually in the Klamath River below Upper Klamath Lake, posing a threat to endangered species [25]. SOD was studied in the Pasig River in the Philippines which came to a profound conclusion of algal respiration is the main contributor to the increase of SOD [26]. Ayers Island Reservoir, Franklin Dam, and Eastman Falls all demonstrated a similar trend in another case study examining sediment-water column exchange outcomes that resulted in a rise in the level SOD [27]. Other research based on the SOD concept was performed for the Lake Yuan-Yang situated in central Taiwan, in that study many undisturbed samples were taken from the core of the river and later tested at the laboratories for SOD values, and based on the WASP program a three-dimensional water quality model was developed, the model that simulated the lake's dissolved oxygen distribution, and when it was calibrated it was found that the model was an exact replicant of the dissolved oxygen DO concentrations at the field [28].

1.1.3 Nitrogen in waters: Forms and concerns

Nitrogen N is one of the most widely found elements in both ground and surface waters, and it may be found in one or more of its various chemical forms almost anywhere on the surface of the earth, but when N concentrations are high, the sources are usually linked to human activity in many cases, nitrogen enters the water in a variety of ways, in the inorganic form: ammonia, ammonium, nitrate, and nitrite and the organic state would be: proteins, amino acids, urea, live or dead organisms such as algae and bacteria, and the process of decomposing plant material can be considered a rich source of N organic. The forms of measuring N are two common techniques: the first is known as the total Kjeldahl nitrogen TKN which is based on determining the organic N it is composed of organic N and ammonia+ammonium. There are many factors influencing the availability of organic N in water bodies, the most common is the distance and point of impact for pollution sources [29]. In the northern region of the Chinese surface water, it was concluded through research study that the pollution of surface water was due to the excessive application of fertilizers which affected the level of nitrogen in the ecosystem [30]. At the Supral river, many observation stations are fixed to measure the changes in levels of nitrogen and phosphorus, it was concluded from the results that the rise in nitrogen concentration was related to a specific period when there was a

discharge of a pollutant to the river [31]. An important note to establish is the water column nutrient ratio or total nitrogen TN to total phosphorus TP ratio (TN: TP) and identifying the ratio of these nutrients combined would provide accurate information on nutrient limiting and the influence it exerts upon the phytoplankton growth [32], this result was also proven for Lake Victoria [33].

1.1.4 Phosphorus effect on surface water quality

Phosphorus is an essential nutrient element in the ecosystem, however, the increasing availability of the nutrient may trigger outbursts of algal blooms, a well-known phenomenon as eutrophication the latter condition will severely affect the ecosystem and other forms of life, and the overall status will be a decrease in the dissolved oxygen level due to periods of algal respiration and breakdown [34]. Another negative status resulting from eutrophication is unacceptable taste-and-odor incidents such as in the case of the Tulsa water supply system at Spavinaw Reservoirs, Oklahoma [35]. A crucial point to notice is the correlation between non-point watershed nutrient of type phosphorus loss and total phosphorus nutrient entering the lake system [36]. This was evident in Washington's Liberty Lake ecosystem, the researchers concluded that the influential nutrient is phosphorus, and through the process of diffusion, they are moving from the bottom sediment to the overlying water, maintaining oxidizing conditions at the sediment surface [37]. Another study linked phosphorus release from sediment with nutrient limitation in the water column as part of reservoir management, as the author focused on internal mechanisms that contributed significantly to the increase of eutrophication, the research went further to elaborate that in the case of phosphorus release from the sediments due to anoxic conditions may alter the TN: TP ratio and concentrations [38].

1.1.5 Affect of Algal abundance on surface water quality

The interaction among the factors influencing the eutrophication process is still not fully comprehended, having said that many available tools and models simulate algal bloom may predict chlorophyll-a concentration as part of the water quality management, these models also include simulation of hydrology, land use,

and biotic interactions, a research was carried out to measure concentrations of chlorophyll through the control of phosphorus and the amount of nutrient entering the tropical reservoirs is just as critical as it is in temperate ecosystems [39]. In a sense using alternative methods to collect data for simulating water quality models by utilizing remotely sensed observations that can aid to increase considerably our understanding of water quality as in the case of Arizona reservoirs which were evaluated by algal abundance and particle loading, the author proved the usefulness of the remote sensing technique, especially when applied over extended periods [40].

1.1.6 Thermal stratification of water bodies

Vertical stratification of masses occurs in water bodies: lakes, ponds, and water supply reservoirs, the important factor regarding the density differences aid in the stratification process however, the changes caused by differences in temperature and dissolved chemicals provided thermal stratification which occurs throughout the warm season, on the contrary during the cold season, surface cooling forces vertical water circulation, resulting in a phenomenon known as turnover this yearly cycle spends more time in late summer and early fall in warmer climates, the important concept for water management is that stratification causes a decrease in the availability of dissolved oxygen levels, this situation will result in the death of many organisms and the algal bloom and deterioration of the water quality [41]. In the case of Lake Tahtali, it was evident that meteorological conditions and factors such as variations in air temperature, wind speed, humidity, and turbidity are all associated with the rise of dissolved oxygen level and thus the water quality [42]. The Keban dam reservoir, also known to be the second-biggest dam in the Euphrates basin, was studied comprehensively. It was sought that between June and August, temperature stratification was found at the reservoir, and epilimnion occurred up to a depth of ten meters, whereas the hypolimnion occurred below, the research work-study had unveiled a correlation between physicochemical characteristics and the water column [43]. A two-dimensional model of DO distribution in the Laurentian Channel bottom had been constructed to capture the cumulative effect of a significant sediment oxygen demand along the estuary [44].

1.1.7 Eutrophication of water bodies

When a water body is impacted by levels of nutrients mostly nitrogen and phosphorus exceeding the acceptable levels this will lead to a well-known condition of eutrophication or an algae bloom. As the nutrients enter the system the trophic condition starts to change, and it shifts from mesotrophic to a eutrophic phase however when there is a decline in the nutrient influx the status will shift in the opposite spectrum of conditions. The eutrophication increased level is due to the increase in human activities which increased the contamination level in the environment, summer algal blooms are the most visible sign of eutrophication, in lakes and reservoirs, however outbreaks and increased growth of algal blooms disadvantage in the: decrease in recreational use of the reservoir, aesthetic issues and damage to the units at the water plant facility. Eutrophication state of the reservoir increase concentrations of organic suspended particles and toxins in water as well as oxygen deprivation leading to changes in raw water quality features, and thus increasing the cost of water treatment [45]. An extensive study was carried out on the Enxoé reservoir in southern Portugal the findings of the research were very interesting as the reservoir's principal contributor to the eutrophication was not from an external source but from the internal processes that caused the release of phosphorus from deposited sediment under anoxic conditions [46]. In the Turkey dam reservoir of Keban, the authors managed to develop a three-dimensional hydrodynamic model that simulated the water quality of the reservoir's complicated water body dynamics, eventually, following calibration and verification the model was utilized to predict dissolved oxygen and euphotic chlorophyll-a concentrations under various conditions and thus, plan the best strategy to eliminate the source of pollution and minimize damage to the system [47].

1.2 Statement of the problem

Monitoring data is the preferable source of information for identifying contaminated waterways for a variety of reasons [48]:

- In some cases, modeling may be viable where monitoring is not.
- For the same overall cost, integrated monitoring and modeling systems might deliver greater information than either one alone.

- Modeling is used to plan out the future condition for the system as part of an overall management strategy plan system. For the Kurtboğazi dam reservoir, a quality model was developed in this effort. Temperature, nitrate, dissolved oxygen, ammonium, chlorophyll a, total phosphorus, total Kjeldahl, and biological oxygen demand (BOD) were included as state variables in the model. Based on the calibrated quality model established, a diagenesis sediment oxygen demand SOD model was simulated and later used to investigate the correlation of SOD with other state variables for the dam reservoir. The model was calibrated with real data from the site and checked using statistical tests. However, the variation in DO in rivers is produced by the action of either oxygen sources or sinks, the main sources of DO are atmospheric re-aeration and photosynthesis, oxygen requirement in sediments in addition to aquatic plant respiration, and the oxidation of Sediment Oxygen Demand SOD is a primary oxygen sink because it includes both the chemical oxidation of reduced compounds in the sediment and organic molecules and other reduced matter in the water column. SOD contributes significantly to oxygen depletion, can make up a significant portion of the total oxygen demand in some water systems, and is crucial for maintaining water quality.

1.3 Scope of Work

This study aims to present the application of the WASP8 water quality simulation program for Kurtboğazi dam reservoirs and give information about sustainable reservoir management. Chapter one displays the introduction to the water quality of a reservoir and related previous research efforts of other authors that are related to this issue of quality management for reservoirs. The second chapter of this study is allocated for describing the methods used for the model that is used in this research, accompanied by a model application. The WASP8 software was used in the third chapter to simulate a reservoir utilizing all hydrodynamic model findings and the following state variables: temperature, all hydrodynamic model findings and the following state variables: temperature, nitrate, dissolved oxygen, ammonium, chlorophyll a, total phosphorus, total Kjeldahl, and biological oxygen demand. A sediment oxygen demand (SOD) diagenesis model was developed based on the quality model to examine the relationship between SOD and other state variables at the reservoir. Calibration of this model was accomplished using data from the actual site, followed by statistical application to ensure the water quality simulation model accurately represents the actual case of the Kurtboğazi reservoir. The conclusions of this work are presented in chapter four, followed by references and appendices.

CHAPTER 2

METHODOLOGY

2.1 Characteristics of the study area

Kurtboğazı dam is still used for drinking water and irrigation today, in addition to functioning as a recreational facility, the General Directorate of State Hydraulic Works DSI is Turkey's principal executive state agency in charge of the nation's entire water resource planning, management, execution, and operation. The primary goal of DSI is to develop all of Turkey's water and land resources, as it seeks to make the best use of the available natural resources.

In 1972 the reservoir was built on the Kurtboaz dam, it is located about 25 kilometers from the Kizilcahamam district and 40 kilometers northwest of Ankara in the Central Anatolia Region a terrestrial climate is predominant; it is worth mentioning that the summers are hot and dry, while winters are chilly and wet with spring being the rainiest season, and July and September are the driest, the dam has a considerable water surface and is one of the few sites with great recreational possibilities in Ankara with green surroundings, two main streams are feeding the Kurtboğazı Dam, Kurt Stream is known to be one of them the other is Pazar Stream [4], Figure 2.1. Ankara metropolitan municipality, the directorate general of Ankara water and sewage administration ASKI provides treatment facilities that are regularly checked in ASKI water quality control laboratories, by analyzing water samples taken from many points determined in various districts of Ankara, to ensure that all standard requirements with both the ministry of health regulations and world health organization are achieved for a water quality that is potable in the quality and quantity measures. Due to the importance of the Kurtboğazı dam reservoir as a source of water supply to Ankara, the General Directorate of State Hydraulic Works-DSI along with the General Directorate of Ankara Water and Sewerage Administration ASKI had

launched many programs to monitor the surface water quality of Kurtboğazi reservoir to protect, improve and ensure sustainable use of reservoir, it had implemented a special conservation plan [50].

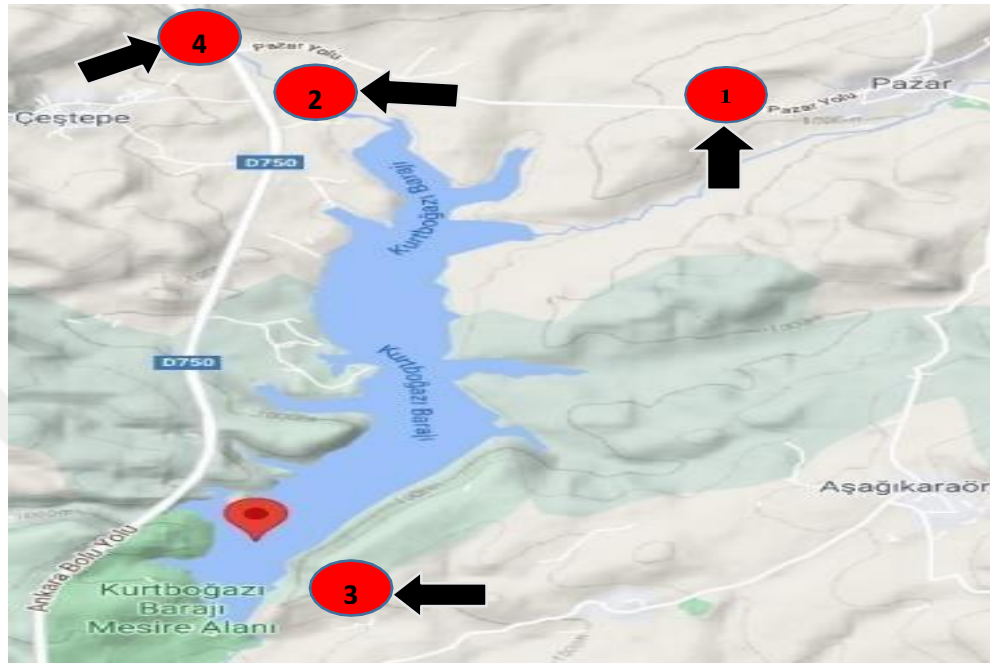


Figure 2.1 Location of study area Kurtboğazi dam reservoir Ankara/ Turkey [50]

FIGURE LEGEND

- 1 Point-1 location of Pazar Stream-Feeding to Kurtboğazi reservoir
- 2 Point-2 is where the Kurt Çay Stream-Feeding to Kurtboğazi reservoir
- 3 It is the discharge point of Kurtboğazi reservoir
- 4 The discharge for Water derived from Eğrekkaya dam to

2.2 Constructing Water Quality model for Kurtboğazi Dam Reservoir

Flowing water in a reservoir experiences a range of physical and chemical changes that might impact the quality of fish habitat both inside the reservoir and downstream. The magnitude of the changes is related to the reservoir's water retention period, which is defined by the reservoir's storage capacity with the watershed size and precipitation length, the deterioration of reservoir water quality may be varied and it is affected by the dissolved gases and temperature, however, aquatic life need dissolving oxygen to flourish, and temperature determines biotic development rates, therefore, temperature and dissolved gases both have an impact on various physical qualities of water, as well as chemical reactions, in general enrichment of phosphorus and nitrogen, in particular fosters excessive primary production, which can deplete oxygen. Although early stages of eutrophication appear to benefit fish development and biomass and appear to be advantageous from a fisheries standpoint, water-quality changes associated with higher trophic states may include hypoxia, and denser phytoplankton blooms, reduced water clarity, and other factors. Eutrophication is the process of increased nutrient enrichment, particularly phosphorus and nitrogen, which produces phytoplankton blooms deteriorate water quality, and causes changes in the ecosystem. The Environmental Protection Agency known as USEPA is an independent executive agency of the United States federal government assigned with environmental protection matters, had created the Water Quality Analysis Simulation Program WASP to simulate water quality in one, two, or three dimensions rivers, lakes, estuaries, coastal wetlands, and reservoirs, the WASP is a time-varying model that may be used in conjunction with hydrodynamic and sediment transport models to compute flows, velocities, temperature, salinity, and sediment fluxes [7]. During model application, the boundary conditions, loads, mass transfer rate, kinetic rates, and concentrations of organic compounds, trace elements, and phytoplankton are required, and the output is a range of concentrations. In a network of branching streams or shallow rivers, the WASP streamflow model uses a set of one-dimensional equations to determine water flow and volume. However, water velocities and flows are calculated through the application of the equations of motion, which are based on the conservation of energy. This network may include kinematic wave flow.

Free-flowing stream reaches, ponded reaches, weir overflow, and backwater or tidally affected lengths dynamic flow. In a network of branching streams or shallow rivers, the WASP streamflow model uses a set of one-dimensional equations to determine water flow and volume [7]. Water flow across a given computational network drives effective transport, internal flows advect most elements along defined flow pathways through the network and out the downstream borders, whereas inflows bring boundary concentrations into the network. The WASP kinetic models are based on a set of transport and transformation equations Figure 2.2. Conservation of mass forms the basic fundamental foundation of the water quality analysis simulation program WASP theory, as the simplest form of writing the mass balance equation, would be:

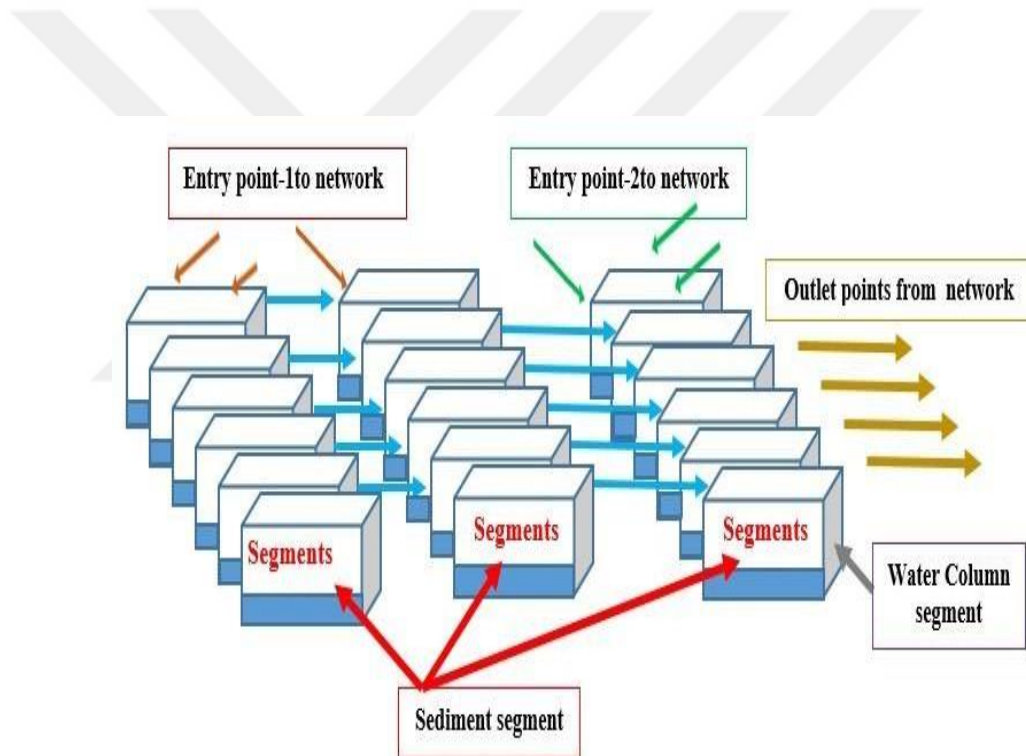


Figure 2.2 Water flow through specified segments in a network

$$\text{Input to the system} + \text{production} = \text{output from the system} \quad (\text{Eq. 1})$$

A lake or river can be considered as a tank reactor and based on eq. (1) therefore mass balance equation:

$$Q_0 \cdot C_{A,0} + r_A \cdot V = Q \cdot C_A + \frac{dn_A}{dt} \quad (\text{Eq. 2})$$

Q_0 = Inflow ($L^3 T^{-1}$), Q = Outflow ($L^3 T^{-1}$), $C_{A,0}$ = concentration of (A) inflow ($M L^{-3}$), C_A = concentration of (A) in outflow ($M L^{-3}$), r_A = rate at which substances are produced, V = volume (L^3), $\frac{dn_A}{dt}$ = the number of moles of a substance A.

The concentration of the water quality constituent in Cartesian coordinates produces a three-dimensional advection fluid flow-diffusion distribution of pollutants from higher concentration to lower concentration region equation [51]:

$$\frac{\partial C}{\partial t} = -\frac{\partial U_x C}{\partial x} + \frac{\partial}{\partial x} \left(E_x \frac{\partial C}{\partial x} \right) - \frac{\partial U_y C}{\partial y} + \frac{\partial}{\partial y} \left(E_y \frac{\partial C}{\partial y} \right) - \frac{\partial U_z C}{\partial z} + \frac{\partial}{\partial z} \left(E_z \frac{\partial C}{\partial z} \right) + S_L + S_B + S_K \quad (\text{Eq. 3})$$

C = quantity amount of concentration of the constituent ($M L^{-3}$), t = time (T), U_x , U_y , U_z = longitudinal, lateral, and vertical advective velocities ($L T^{-1}$) and E_x , E_y , E_z = longitudinal, lateral, and vertical diffusion coefficients ($L^2 T^{-1}$), S_L = direct and diffuse loading rate ($M L^{-3} T^{-1}$), S_B = boundary loading rate (including upstream, downstream, benthic, and atmospheric) ($M L^{-3} T^{-1}$), S_K = total kinetic transformation rate; positive is a source, negative is a sink ($M L^{-3} T^{-1}$). The term budget calculation explains how the mass balance equation is used to compare input and output data involved in environmental monitoring in eq. (1) emphasizes that any mass entering a system must, by conservation of mass, either accumulate within the system or exit the system, is also Completely Mixed Flow Reactors (CMFRs) properties may be assumed, which means control volumes for spatially uniform:

$$\text{Accumulation} = \Sigma \text{imports} - \Sigma \text{exports} + \Sigma \text{sources} - \Sigma \text{sinks} \quad (\text{Eq. 4})$$

$$\text{Accumulation} = \frac{\text{amount at } (t+dt) - \text{amount at } (t)}{\text{duration } dt} = \frac{V C(t+dt) - V C(t)}{dt} = \frac{d(V C)}{dt} = V \frac{dc}{dt} \quad (\text{Eq. 5})$$

$$\Sigma \text{ Imports} = \Sigma_{\text{inlet}} \frac{\text{mass}}{\text{volume}} * \frac{\text{volume of carrying fluid}}{\text{time}} = \Sigma_{\text{inlet}} C_{IN} * Q_{IN} \quad (\text{Eq. 6})$$

$$\Sigma \text{ Exports} = \Sigma_{\text{outlet}} \frac{\text{mass}}{\text{volume}} * \frac{\text{volume of carrying fluid}}{\text{time}} = \Sigma_{\text{outlet}} C_{OUT} * Q_{OUT} \quad (\text{Eq. 7})$$

Σ Sources= to be specified on each case application Σ Sinks= Decay constant \cdot amount

$$\text{present} = K \cdot V \cdot C \quad V \frac{dc}{dt} = \Sigma_{\text{inlet}} C_{\text{IN}} \cdot Q_{\text{IN}} - \Sigma_{\text{outlet}} C_{\text{OUT}} \cdot Q_{\text{OUT}} + S - KVC$$

V = control volume (L^3), C = concentration of substance ($M L^{-3}$), Q = volumetric flux of fluid ($L^3 T^{-1}$), S = sum of emissions and K = decay constant. Therefore by re arranging the above equations:

$$\frac{\Delta(V_i C_i)}{\Delta t} = \Sigma_j Q_{j,i} C_j - \Sigma_k Q_{i,k} C_i + \Sigma_j \frac{E_{i,j} A_{i,j}}{L_{i,j}} (C_j - C_i) + S_{L,i} + S_{B,i} + S_{K,i} \quad (\text{Eq. 8})$$

j are pointers to either a boundary or adjoining segments, Q = advective flowrate ($L^3 T^{-1}$), E = dispersion coefficient ($L^2 T^{-1}$) across an interface, A = interfacial area (L^2), L = the characteristic length (L) and V = control volume (L^3), C = concentration of substance ($M L^{-3}$), t = time (T), $S_{L,i}$ = direct and diffuse loading rate ($M L^{-3} T^{-1}$) $S_{B,i}$ = boundary loading rate (including upstream, downstream, benthic, and atmospheric) ($M L^{-3} T^{-1}$), $S_{K,i}$ = total kinetic transformation rate; positive is a source, negative is a sink ($M L^{-3} T^{-1}$).

Model functions under the principle of completely mixed finite segment or integrated control volume using eq. (8) [51]:

$$\frac{\Delta(V_i C_i)}{\Delta t} = \Sigma_j Q_{j,i} C_j - \Sigma_k Q_{i,k} C_i + \Sigma_j \frac{E_{i,j} A_{i,j}}{L_{i,j}} (C_j - C_i) + S_{L,i} + S_{B,i} + S_{K,i} \quad (\text{Eq. 9})$$

The rate of mass change for components is determined by dispersive and advective movement across the system, which is referred to as imports and exports, as shown in eq. (9), all external loadings or sources on the system, as well as chemical energy, have been transformed into kinetic energy; total kinetic transformations are included in this phrase. The coupling modeling of physical and biochemical processes provides a powerful tool for assessing quantitatively the water quality in a water body, and the water quality model used in this study was built based on a three-dimensional traditional water quality analysis simulation program WASP8 developed by the authors [51]. This program includes eight water quality components such as dissolved oxygen DO, phytoplankton chlorophyll-a, the BOD or the biochemical oxygen demand, NH_4 , nitrate, nitrite, inorganic phosphorus, organic nitrogen, and organic phosphorus in a system that is not only complex but also involves the reaction of

separate cycles and systems: phytoplankton dynamics, nitrogen cycle, dissolved oxygen and phosphorus cycle, the mathematical formulation of the conservation of mass can be written [50]:

$$\frac{\partial C}{\partial t} + \frac{\partial(uC)}{\partial x} + \frac{\partial(vC)}{\partial y} + \frac{\partial(wC)}{\partial z} = \frac{\partial}{\partial x} (A_u \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} (A_u \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z} (K_v \frac{\partial C}{\partial z}) + S_c \quad (\text{Eq. 10})$$

C is the concentration of the water quality components; u, v, and w are the water velocity components corresponding to the Cartesian coordinate system (x, y, z); A_u and K_v are the coefficients of the horizontal viscosity and vertical eddy diffusion, respectively;

S_c is the function that represents the internal source or sinks of the horizontal viscosity and vertical eddy diffusion, respectively; C is the concentration of the water quality components; u, v, and w are the water velocity components corresponding to the Cartesian coordinate system (x, y, and z); and S_c is the function that represents the internal sources or sinks of the water quality component. One source of dissolved oxygen (DO) in the water column is photosynthetic carbon fixation, which is related to the phytoplankton population and development rate. Other activities related to SOD, phytoplankton respiration, nitrification, and the oxidation of carbonaceous biochemical oxygen demand (CBOD) typically reduce the value of DO in the water column.

Dissolved oxygen, or DO, is the first element to consider when assessing water quality. Photosynthetic carbon fixation, which is related to phytoplankton population and growth rate, is one source of DO in the water column. Other activities related to SOD, phytoplankton respiration, nitrification, and the oxidation of carbonaceous biochemical oxygen demand, or CBOD, typically result in a decrease in DO levels in the water column. The mathematical representation that links transport processes with biogeochemical cycles [51]:

$$S_c = K_{r1} \theta_{r1}^{(T-20)} (C_S - C_{DO}) - K_{d1} \theta_{d1}^{(T-20)} \frac{C_{DO} * C_{CBOD}}{K_{BOD} + C_{DO}} - \frac{32}{12} K_{r2} \theta_{r2}^{(T-20)} C_{Phyt} - \frac{32}{12} 2K_{ni} \theta_{ni}^{(T-20)} \frac{C_{DO} * C_{NH4}}{K_{NITR} + C_{DO}} + G_P [\frac{32}{12} + \frac{48}{14} a_{nc} (1 - P_{NH4})] C_{Phyt} - \frac{SOD_T}{D} \quad (\text{Eq. 11})$$

a_{nc} is the Phytoplankton nitrogen-carbon ratio; C_S is the DO saturation

concentration; CDO, CCBOD, CNH₄, and CPHYT are the DO, CBOD, NH₄, and phytoplankton concentrations respectively; D is the depth of the benthic layer; GP is the phytoplankton growth rate; K_{r1} is the reaeration rate; K_{d1} is the CBOD deoxygenation rate; K_{ni} is the nitrification rate; K_{r2} is the phytoplankton respiration rate; K_{BOD} is the half-saturation concentration for the oxygen limitation of CBOD oxidation; K_{NITR} is the half-saturation concentration for the oxygen limitation of nitrification; P_{NH4} is the ammonium preference factor; SODT is the sediment oxygen demand at T °C; Θ_{r1} the temperature adjustment for the reaeration rate; Θ_{d1} is the temperature adjustment for the deoxygenation rate; Θ_{ni} is the temperature adjustment for the nitrification rate; Θ_{r2} is temperature adjustment of phytoplankton respiration rate eq.(11) provides the vertical distributions of nutrients and phytoplankton, but it is also well known that nutrient fluxes from sediment to the water column are frequently an important source of nutrients for primary productivity in eutrophic lakes. Bottom sediments, the water column, and seasonal variations all have a connection [52]. Our modeling effort aims to incorporate state variables that directly affect water quality: phytoplankton properties of respiration, growth, mortality, and settling. Phytoplankton biomass is acknowledged as a fundamental indication of the trophic status in a water body.

The kinetic equations used in this work, as well as those used in the WASP8 water quality model created for the United States, are the same for the mineralization of organic phosphorus, organic nitrogen, nitrification, denitrification, particulate BOD settling, oxidation of carbonaceous and nitrogenous material, changes in DO concentration due to reaeration, oxidation of organic matter, nitrification, and sediment oxygen demand. (USEPA) [47].

2.2.1 Oxygen demand and different levels of complexity

Dissolved oxygen levels in the system are mainly influenced by many factors such as nitrate, phytoplankton, ammonia, nitrate, and biochemical oxygen demand. In other words, two major activities one of them taking place due to the aerobic respiration activity that results in oxygen decrease, or respiration for the aerobic system, and the activities at the water column which involve anaerobic reactions can

be expressed in the following:

1- Streeter-Phelps: The Streeter-Phelps BOD-DO equations [7]:

$$S_{k5} = -K_d \theta_d^{T-20} C_5 - \frac{v_{s3}}{D} (1-f_{D5}) C_5 \quad (\text{Eq. 12})$$

$$S_{k6} = +K_2 \theta_2^{T-20} (C_s - C_6) - K_d \theta_d^{T-20} C_5 - \frac{SOD_T}{D} \quad (\text{Eq. 13})$$

S_{ki} is the source/sink term ($\text{mg L}^{-1} \text{ day}^{-1}$), K_d is the Deoxygenation rate at 20°C , Temperature Coefficient (day^{-1}), C_s DO saturation ($\text{mg O}_2 \text{ L}^{-1}$), f_{D5} Fraction dissolved CBOD, v_{s3} Organic matter settling velocity (m day^{-1}), K_2 Reaeration rate at 20°C , temperature coefficient (day^{-1}), SOD Sediment Oxygen Demand, temperature coefficient ($\text{g m}^{-2} \text{ day}^{-1}$), D =average segment depth (m), C drag coefficient, θ temperature coefficient ($^\circ\text{C}$).

2- The Modified Streeter-Phelps: There are two major parts for the biochemical oxygen demand which are carbonaceous and nitrogenous fractions, Figure 2.3, From eq.(13) the modified mathematical equations are:

$$S_{k1} = -K_n \theta_n^{T-20} (C_1) - \frac{V_{s3}}{D} (1 - f_{D1}) C_1 \quad (\text{Eq. 14})$$

$$S_{k6} = +K_2 \theta_2^{T-20} (C_s - C_6) - K_d \theta_d^{T-20} C_5 - \frac{64}{14} K_n \theta_n^{T-20} C_1 - \frac{SOD}{D} \theta_n^{T-20} \quad (\text{Eq. 15})$$

S_{ki} is the source/sink term ($\text{mg L}^{-1} \text{ day}^{-1}$), K_d is the Deoxygenation rate at 20°C , temperature coefficient (day^{-1}), C_s DO saturation ($\text{mg O}_2 \text{ L}^{-1}$), f_{D5} Fraction dissolved CBOD, v_{s3} Organic matter settling velocity (m day^{-1}), K_2 Reaeration rate at 20°C , temperature coefficient (day^{-1}), sediment oxygen demand SOD, temperature coefficient ($\text{g m}^{-2} \text{ day}^{-1}$), D =average segment depth (m), C_1 nitrogenous biochemical oxygen demand NBOD as expressed as total Kjeldahl nitrogen (TKN, mg L^{-1}), K_n is known as the deoxygenation rate constant for nitrogenous (day^{-1}), θ temperature coefficient ($^\circ\text{C}$), f_{D1} is the dissolved fraction of the nitrogenous biochemical oxygen demand.

3. Full DO Balance: These equations divide the NBOD process into mineralization and nitrification, and add the effects of photosynthesis and respiration from given phytoplankton levels Figure 2.4:

$$S_{k6} = +K_2 \theta_2^{T-20} (C_s - C_6) - K_d \theta_d^{T-20} C_5 - \frac{64}{14} K_{12} \theta_{12}^{T-20} C_1 - \frac{SOD}{D} \theta_s^{T-20} + (k_{1c} \theta_{1c}^{T-20} - k_{1R} \theta_{1R}^{T-20}) \frac{32}{12} C_4 \quad (\text{Eq. 16})$$

The term K_{1C} average phytoplankton growth rate constant (day^{-1}) and S_k is known to be either the source or the sink term for variable in a segment in ($\text{mg L}^{-1} \text{ day}^{-1}$) kinetic rate constants and coefficients, Θ temperature ($^{\circ}\text{C}$), K is the rate constant for organic nitrogen mineralization (day^{-1}).

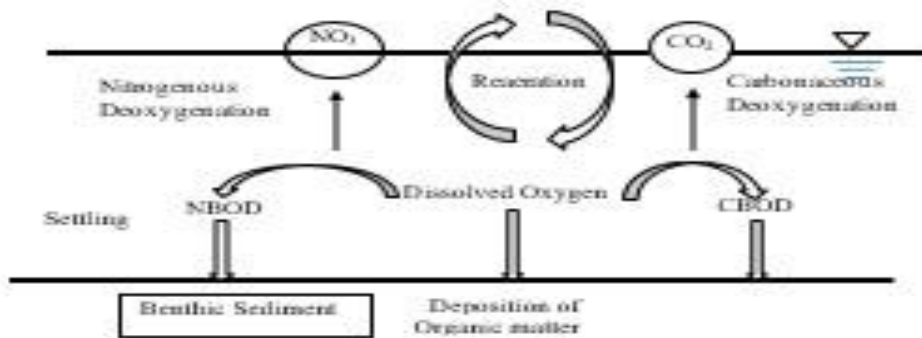


Figure 2.3 Sketch of Modified Streeter Phelps [53]

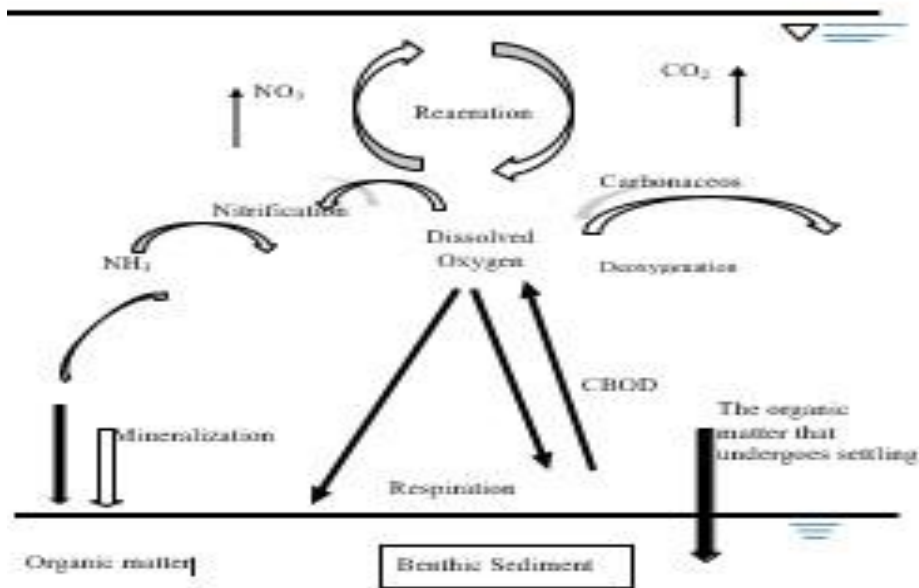


Figure 2.4 Sketch of Full DO Balance [53]

2.3 Application of WASP8 model on Kurtboğazi Dam Reservoir

Field data were collected at specific locations at the monitoring stations in the Kurtboğazi dam [49], Physicochemical properties of water at the stations were provided such that: K1, K2, K3, K4, and K5. For one year which included the surface and sediment analysis at some stations, the simulation program WASP8 is generally based on the principle of mass conservation in eq. (10), this principle requires that each mass constituent being investigated must be accounted for, and the model traces each water quality constituent from the point of spatial and temporal input to its final point of export, conserving mass in space and time, to accomplish this task there are important input data that must be defined by the user: Simulation and output control, model segmentation, advective which is the transfer of matter initial concentrations, boundary concentrations, waste loads, kinetic parameters, and constants. The simulation model tracks the movement and transformation of environmental parameters that are involved in the interaction of the Kurtboğazi reservoir, these parameters are biological oxygen demand BOD which is the quantity of oxygen required by bacteria and other microorganisms when the decomposing organic matter under aerobic oxygen present conditions at a specific temperature are referred to as biochemical oxygen demand BOD [53]. We cannot perceive oxygen when we gaze at a body of water in some ways we think of water as the polar opposite of air, although the average lake or reservoir contains trace amounts of oxygen in the form of dissolved oxygen, high levels of dissolved oxygen indicate a healthy water body [53].

All plants and animals require nutrients to survive and thrive, and these nutrients are in the form of nitrogen and phosphorus, but when the quantity of that nutrient exceeds a certain limit it will have a negative impact on the environment. Nitrogen is a nutrient that plants require in the form of nitrate, nitrite, or ammonium. Nitrogen gas makes up around 78 percent of the air we breathe, all aquatic species expel waste, and all aquatic plants and organisms perish, these actions produce ammonia some bacteria in the water turn the ammonia into nitrite, which is subsequently transformed into nitrate by other bacteria. Nitrates NO_3 are an oxidized form of nitrogen generated by the reaction between oxygen with nitrogen, although nitrates exist naturally in soil and water, high quantities of nitrates can be considered ground

and surface water pollution, the majority of excess nitrates are caused by human activities and excess nitrates are mainly caused by agricultural activity, human waste, or industrial pollution [54]. A cycle of continuous activities in which nitrogen moves through both living and non-living substances, including the atmosphere, soil, water, plants, animals, and biological entities that are typically only one cell in size and are found everywhere. Organic matter in soils may decompose or break down as a result of bacteria, and nitrogen must change forms to go through the cycle's many stages of fixation or volatilization, mineralization, nitrification, ionization, and denitrification. Volatilization is the process by which soil microorganisms turn nitrogen gas N_2 into volatile ammonia NH_3 , whereas leaching is the process by which some nitrogen compounds dissolve in water and seep out of the soil, potentially contaminating rivers. [55]. The bacteria in question are known as Nitrosomonas and Nitrobacter. Some bacteria may convert ammonia to nitrites, though nitrite is not directly used by plants or animals, while other bacteria may convert nitrites to nitrates, which are usable by plants and animals. This reaction provides energy to the microorganisms involved in the process. The fourth step in the nitrogen cycle is immobilization, which is sometimes referred to as the reverse of mineralization. Nitrobacter converts nitrites to nitrates whereas Nitrosomonas converts ammonia to nitrites. Both species of bacteria can only function in the presence of oxygen [56]. At the fifth stage of the nitrogen cycle, when nitrates are transformed by bacteria into atmospheric nitrogen N_2 , a process known as denitrification, nitrogen returns to the atmosphere in the form of gas. The method used to calculate the quantitative value of nitrogen included in organic substances in addition to the nitrogen present in the inorganic compounds ammonia and ammonium is known as Total Kjeldahl nitrogen, as shown in Figure 2.5 in the nitrogen cycle. (TKN) [57].

To grow aquatic environments require nutrients such as phosphorus, which is considered a crucial mineral for the aquatic food web, which can be found in water in a variety of forms; it can be dissolved, bound to soil and other particles, or stored within the living or dead plants and animals, plants and algae can easily use dissolved phosphorus, which is typically found in small amounts in unpolluted water bodies; since phosphorus is needed by phytoplankton, including algae [58].

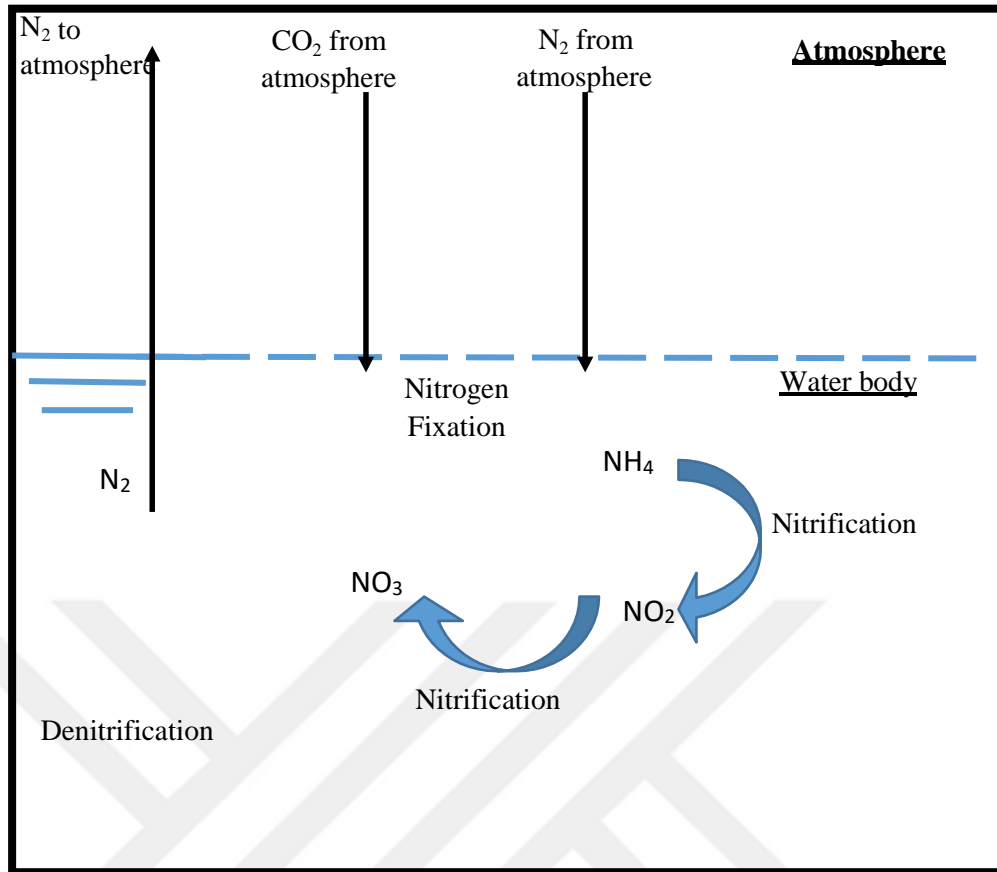


Figure 2.5 Nitrogen cycle [58]

Since TP fluctuations have an impact on algae growth and water clarity, which affect swimming, boating, fishing, and aesthetic enjoyment, phosphorus may be thought of as the foundation of the food web, supporting higher species such as zooplankton, crustaceans, tiny fish, and top predators. However, the concentration of nutrients in a lake or reservoir varies based on its depth, temperature, and other factors. There are numerous other factors at work, including the geology of the rock and soils, the hydrology of water movement, and the naturally occurring presence of phosphorus in sediments in the form of internal loading. Phosphorus levels are frequently higher in the spring due to snowmelt from rivers and streams, which transports nutrients into lakes, and during the spring and summer phytoplankton species consume some of the phosphorus, the system also takes nitrate NO_3 and ammonium NH_4 into account if the water body has exceeded limits for NO_3 and NH_4 , this will eventually cause eutrophication and plant bloom, which depletes oxygen from the water and negatively impacts the water quality, the overall levels of TP provide reliable information on the

water body quality and trophic state [59]. Another parameter that contributes to the aquatic quality is phytoplankton determined as Chlorophyll a, usually, Chlorophyll a is found in many forms within the living cells of photosynthetic organisms such as phytoplankton and cyanobacteria, the quantity of chlorophyll-a present in a water sample is used to calculate phytoplankton concentration. These metrics help to understand the system's overall biological "health," such as its trophic status or primary production [60].

Chlorophyll measurements can also be used to predict hazardous algal blooms and detect algal bloom episodes and their consequences on water quality, which is a direct way of tracking algal growth and by monitoring chlorophyll levels and ensuring it does not exceed permissible levels that leads to algae bloom [61,62] and since the significant key factor to determine the health state of a water body is dissolved oxygen DO, therefore, it is of paramount importance to include DO in the system. Water bodies absorb oxygen from the atmosphere as well as aquatic vegetation, running water, such as that of a fast-flowing stream, dissolves more oxygen than motionless water, such as that of a pond or lake [63] All aquatic species need to dissolve oxygen (DO) to breathe, and when excess organic materials, like large algal blooms, are broken down by microorganisms, low oxygen levels, or hypoxia, or no oxygen levels, anoxia, may develop. These low oxygen levels are frequently found near the bottom of the water column and affect species that live in the sediments. Because dissolved oxygen levels in some bodies of water fluctuate frequently, seasonally, and even daily as part of the aquatic resource's natural daily ecology, certain sensitive animals may flee, suffer health problems, or even perish as dissolved oxygen levels fall. For this reason, it's considered a crucial water quality indicator [64]. While each organism has its unique DO tolerance range, values below 3 milligrams per liter (mg/L) are typically regarded as dangerous, while waters with levels below 1 mg/L are considered hypoxic and frequently devoid of life. Temperature also affects the oxygen level as more oxygen can be dissolved in cooler water, and salinity affects how much oxygen water can retain, as freshwater holds more oxygen than saltwater does. The partial pressure of oxygen, as well as the degree of saturation, will vary with altitude, in the summer many lakes and ponds have anoxic oxygen-deficient bottom layers due to decomposition processes that

deplete the oxygen [65], as outlined in Figure 2.6. There are also other data requirements to be entered before running the model such as weather details such as air temperature, dew point, wind speed, and solar radiation, for the simulation period from 1/1/2019 to 1/1/2020 [66]. As explained earlier, the model is a set of expanded control volumes, or "segments," that together represent the physical configuration of the water body, these segments are provided to help users interpret and predict water quality responses to natural phenomena and man-made pollution for various pollution management decisions since WASP is a dynamic compartment where individual compartments can interact with each other and undergo dynamic remodeling) for aquatic systems, including both the water column and the underlying benthos [67]. As shown in Figure 2.7 the Kurtboğazi reservoir is divided into 8 segments for the surface layer however these segments will have a subsurface layer below it as part of the water column, also, there is the surface benthic and subsurface benthic that make up the sediment bed, the total number of segments will be 16, for each segment surface and subsurface water dimensions with areas and volumes are given in Table 2.1 and the same concept was also applied to sediment beds for surface and subsurface benthic, based on the segment division in Figure 2.7, the dimensions were derived in length and width and the last two columns are for the area and volume of each segment, as listed in Table 2.1, the dimensions are required to be entered into the model as part of the input procedure.

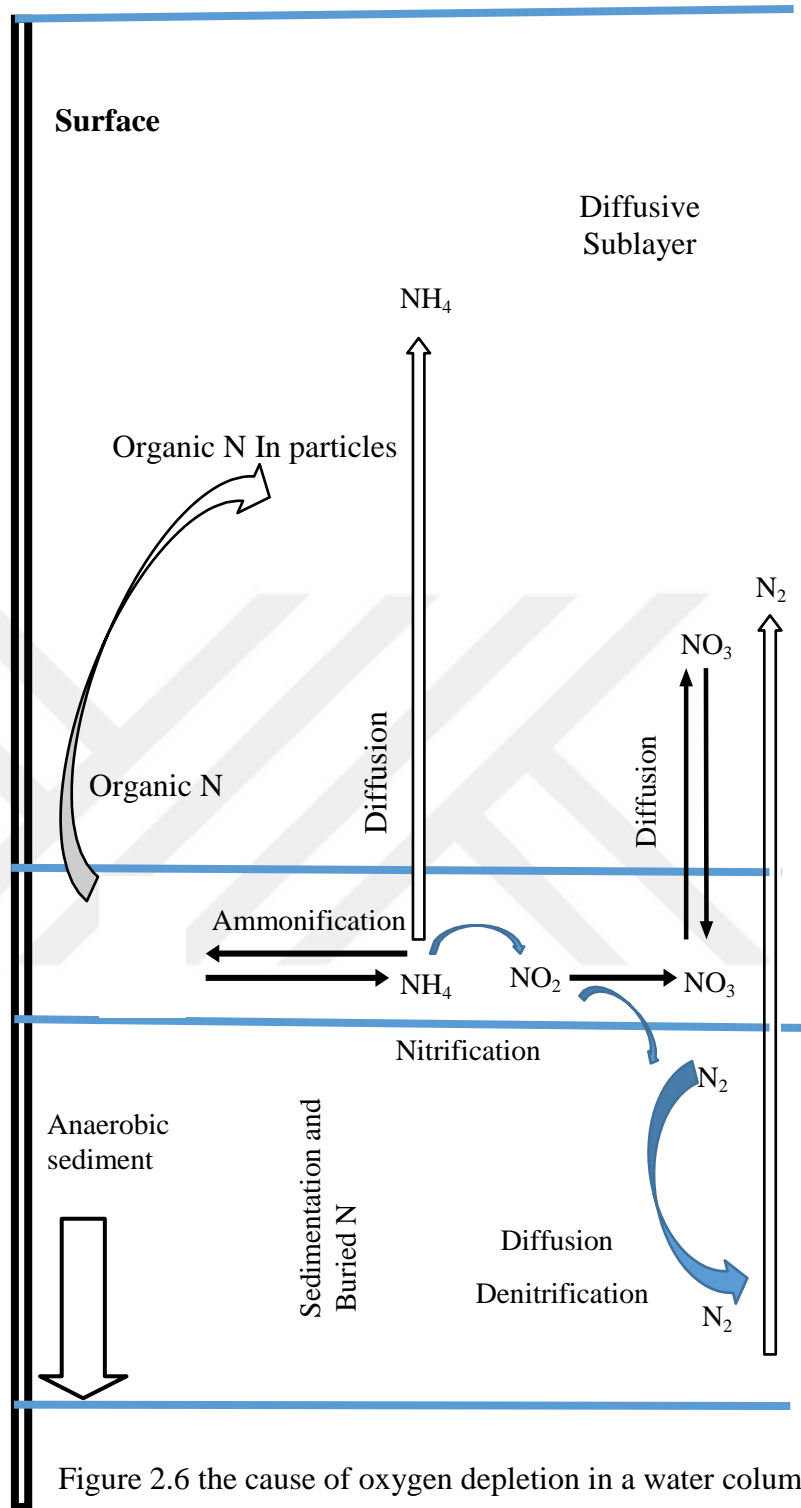


Table 2.1. Dimensions of segments

Name	Length (L)	Width (W)	Area (m ²)= L·W	Volume (m ³) =L·W·depth
1	1136	845	959920	31677360
2	874	816	713184	24248256
3	904	714	645456	20654592
4	1020	670	683400	22552200
5	1224	641	784584	26675856
6	918	568	521424	17206992
7	1064	787	837368	29307880
8	758	685	519230	18173050

2.4 Model setup and application

Our selected simulation period for this work is from 1/1/2019 to 1/1/2020, the reason for selecting this time frame is because the available data that was sent from ASKI was during that period. According to [4], [48], and [49], there are two inlet points as shown in Figure 2.1, Kurtboğazı reservoir known as Kurt and Pazar these will represent segment 1 and segment 2 in the model respectively, the discharge point from the Kurtboğazı outlet location corresponds to segment 8 in the model, the reason for selecting these specific segments is because they correspond to effective location points as inlet and outlet points at the reservoir, as for the remaining observation stations they correspond to segment numbers as presented in Figure 2.7

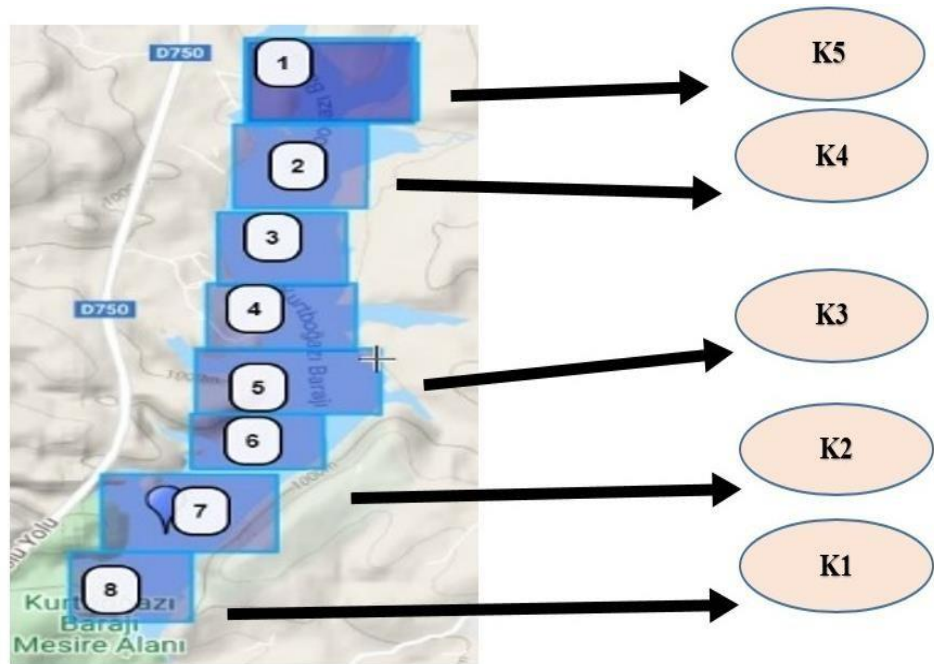




Figure 2.7 Google map of Kurtboğazi reservoir -segments [49]

	From K1 to K5 are locations of measurement stations at the site of Kurtboğazi reservoir
	Along the Kurtboğazi reservoir it was divided into sectors of rectangles in order to calculate the total area for each segment as it's a requirement and part of the input for the simulation model program

Observation stations that are fixed on the site and fixed by the management are given the names: K1, K2, K3, K4, and K5. However on the WASP8 model according to their locations, the observation stations represent segment 8; segment 7; segment 5; segment 2; and segment 1 respectively, as mentioned earlier this work will focus on segments 1, 2, and 8 as they are considered key influencing points in the model and as mentioned earlier. Before being used to calculate the sediment oxygen demand, the chosen mathematical modeling approach underwent a thorough calibration process, with the results of a series of calibration runs being compared with a set of prescribed field measurements. The goal of carrying out calibration trials for predetermined periods was to find an appropriate combination of numerical values for the model parameters and thereby obtain an acceptable, match between mode and mode. Utilizing statistical techniques like root mean square error and restricted regression analysis from Chapter 3, the calibration results were verified.

2.5 Modeling Sediment Oxygen demand SOD

Since sediment-oxygen SOD is a significant cause of hypolimnetic oxygen depletion, SOD rates are crucial indicators of the health of aquatic ecosystems [68]. The basic layout of the sediment model shows two sediment layers that are continuously mixing. A thin top sediment layer called the aerobic layer and a thicker active anaerobic layer make up the surface water column segment, which is also subject to aerobic activity. In WASP, the user can choose the active layer's thickness, which is assumed to be constant across all sediment columns. The sediment model also includes three important processes. [51]:

- Fluxes of particulate natural matter from the water column to the sediments.
 - Process of diagenesis for particulate organic materials.
 - Chemical reactions for movement of matter from the sediment to the water column.
- The materials in sediment are known to be the fluxes of particulate organic matter POM and they are subdivided into particulate organic carbon and particulate organic nitrogen. However, these are further divided into G- classes which are based totally upon their reactivity. WASP calculates settling fluxes for these state variables using the given % dissolved, which varies by segment and state variable, the state variables' particle transport fields, and the stated solids transport rates, particulate organic

carbon in the diagenesis model is quantified in oxygen equivalent units CBOD rather than carbon units as in other models, the flow of algae to the sediment model is partitioned into carbon-oxygen equivalents, nitrogen, and phosphorus using given stoichiometric constants. Internal diagenesis sediment state variables are based on the multi-class G model, which classifies organic forms as reactive-G1, refractory-G2, or inert-G3 depending on their reactivity Figure 2.8, as a consequence, based on user-specified ratios of nitrogen, and phosphorus fluxes are sorted into G-class fractions [51].

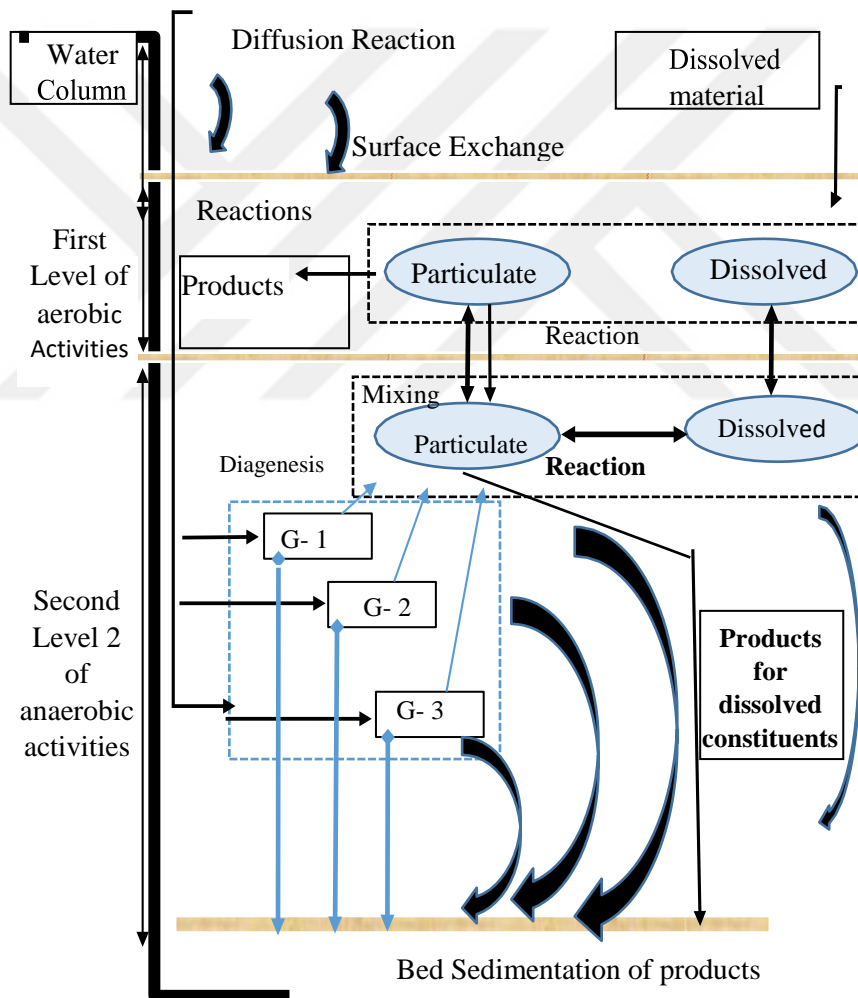


Figure 2.8 Basic structure of the SOD diagenesis column [51].

The sediments absorb fluxes of particulate organic carbon POC, nitrogen PON, and phosphorus POP from the water column, which are referred to collectively as particulate organic matter POM, however, must bear in mind that fluxes in the simulation model of WASP are measured in oxygen equivalents.

Digeneis mineralization processes occur in the second layer of anaerobic sediment, each G class (1-3) has diagenesis equations that are comparable for each particulate organic matter type N, P, and C, to determine time-varying diagenesis for each modeled variable, such as POC, PON, and POP in each G class, a mass balance equation is generated for each form and type of POM, the mass balance equations can be solved algebraically for the present concentration at this time step, however, the diagenesis source terms for reactions and transfers are computed after the current time step concentrations have been computed. After obtaining the sediment particle, organic matter C, N, and P concentrations and source terms for the current time step, computing the reactions and transfers and calculating the contents of ammonia, nitrates, methane, sulfates, sulfides, silica, and phosphorus as well as sediment oxygen demand, the diagenesis source terms for C, N, and P are calculated by adding the chemical-specific reaction velocities and estimated concentrations. Because the surface layer is thin in comparison to the active anaerobic layer, it is possible to infer that layer 1 is in a stable state, as opposed to the slower processes taking place in layer 2, where the layer thickness is believed to remain constant. Total chemical concentrations are calculated using mass balance methods. A matrix solution is used to solve the equations for the new concentrations. Except for phosphates and silica, each of these elements has an impact on SOD, which in turn has an impact on the rate of surface transfer. As a result, an iterative approach is necessary. Sampling these rates, on the other hand, might be too expensive. Additionally, sediment flow to the overlying water column is calculated based on the chemical concentrations in layer 1. [69]. SOD is defined as the rate at which dissolved oxygen is removed from the water column in surface water bodies as a result of the breakdown of organic matter in the sediment, and it encompasses both the chemical oxidation rates and the respiration rates of benthic communities, area, deposit depth, temperature, water velocity, chemical variations, and biological variations. The issue of oxygen

depletion in aquatic ecosystems has received a great deal of attention; in surface water bodies, anaerobic respiration of invertebrates in sediments consume significant amount of and aerobic breakdown of deposited organic materials have been reported to consume a of the water column oxygen [70], whereas aerobic breakdown of organic materials is reported to consume, surface runoff, wastewater effluents, and aquatic conditions are all factors that affect the rate of SOD. Sediments can also have a high oxygen demand due to the preservation of organic material by organisms like bacteria. Benthic algae with strong primary production may also have a high benthic oxygen demand.

Estimating SOD via measuring techniques might be expensive due to regional changes in climates that result in different values of SOD, their rates vary greatly in most surface water systems, both regionally and seasonally, due to varying sediment composition [71]. Deposition, as well as the physical and chemical makeup of sediment layers, all of which affect how much oxygen is consumed in rivers and lakes, varies dramatically over time. Constituents of different sizes settle at the inlet as a river's current slows due to resistance from the lake's relatively still body of water, and sand, silt, and clay are deposited as the current becomes extremely slow beyond the inlet and up to obstructing the flow [72], Changes also have an impact on the make-up of benthic and microbial populations, which restricts the rate of SOD production. Typically, temperature increases have an impact on biological and chemical processes in sediments. As a result of these differences, it's common to need plenty of observations to accurately describe SOD dynamics, and it may be difficult to correlate data to external sources [73]. In Figure 2.9 a conceptual drawing of the SOD and sediment and water column is presented to summarize all the previous information outlined in the above paragraphs. Since there are no available data of laboratory tests for the sediment at the Kurtboğazı reservoir we have first modeled the SOD using the calibrated water quality model developed in this work then for the calibration of the result alternative steps are implemented which are explained below. According to [74], the sediment oxygen demand could be calculated from the total organic carbon TOC using the following equation [74]:

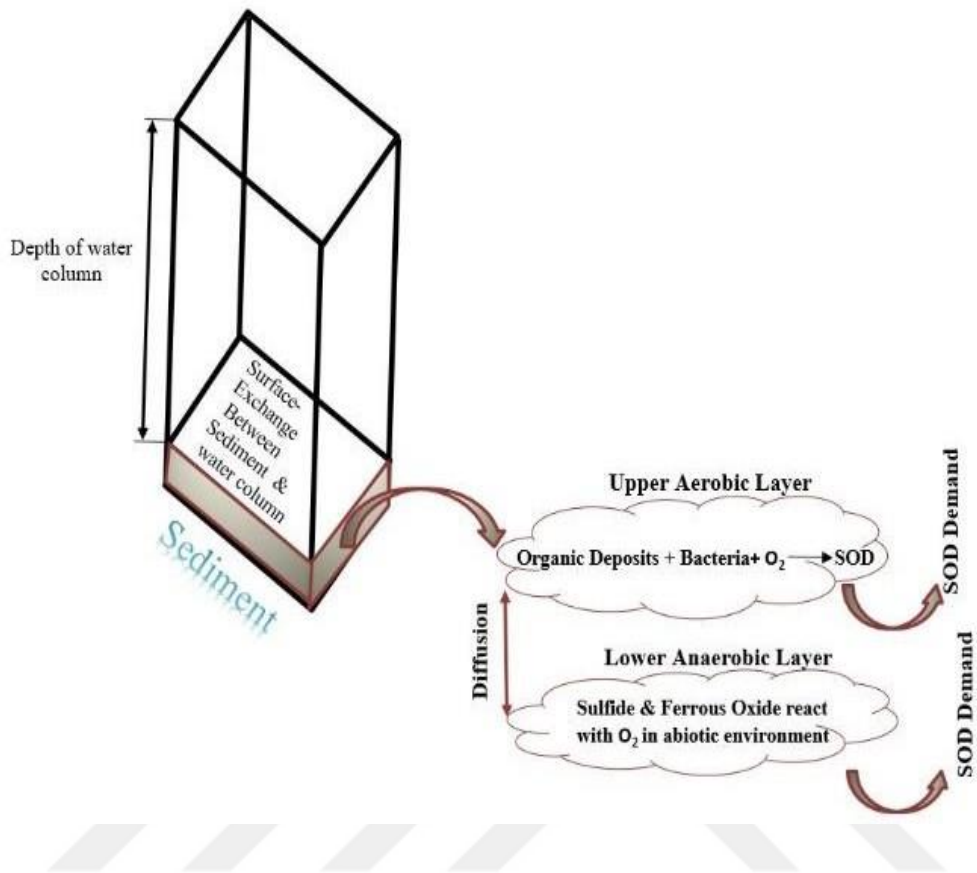


Figure 2.9 Conceptual drawing of SOD between sediment and water column

$$\text{SOD (gm}^{-2}\text{day}^{-1}) = 0.0302 \cdot \text{TOC} + 0.0845 \quad (\text{Eq. 17})$$

Using the result from our model for total organic carbon TOC and applying it to the eq. (17), since TOC is regarded as the most important metric for assessing organic contamination in water [75], the results of segments 1, 2, and 8 are given in Chapter 3.

CHAPTER 3

RESULTS AND DISCUSSIONS

3.1 Kurtboğazı dam reservoir simulation model

The novelty of this work is to do with the fact that this simulation tool has not been used before for the Kurtboğazı reservoir water quality monitoring program, this approach is more pertinent than the conventional known methods used and in reality, according to its capacity, it can combine a few association frameworks comprising biochemical oxygen demand BOD, nitrate, DO, phytoplankton, phosphates, pH, and solids. The fundamental concept of composing a mass adjust condition for a body of water is to account for all the material entering and exiting the water body using coordinate expansion of material runoff and loads, through physical reactions, chemical, and biological changes, and dispersive and advective transport instruments. Our selected simulation period is from 1/1/2019 to 1/1/2020, the reason for selecting this time frame is because the available data that we were able to receive from ASKI is at this period. There are two inlet points in Kurtboğazı reservoir known as Kurt and Pazar [4], [48], and [49], they represent segment 1 and segment 2 in the model respectively, after simulating the system and developing our model, it is essential to ensure that it accurately depicts the real system at the Kurtboğazı reservoir site. As a result, we use field data to calibrate our model results, which will be based on the summer season, Kurtboğazı reservoir is also known as Kurt and Pazar [4], [48], and [49], which present segment 1 and segment 2 in the model, respectively. The reason for selecting this period is due to the fact it is the only available data that we have access to use and the fact that our study focuses on anoxic and oxygen depletion due to stratification and sediment oxygen demand which increase in the summertime, this result was in accordance with other

researchers and previous authors results [76,77], who stated that thermal stratification was mainly controlled by solar radiation and favored the growth of cyanobacteria and led to the release of nutrients from the sediment, threatening the water quality. Table 3.1 presents the simulation result obtained from the WASP8 model for Kurtboğazı reservoir, for the time frame from May 2019 to the end of December 2019 for the state variables: temperature, nitrate, dissolved oxygen, total phosphorus, chlorophyll-a, total Kjeldahl, BOD, & ammonium at segments 1, 2, & 8

Table 3.1 Model results for state variables at segments 1, 2 and 8

State Variable	Segment Number	2019				
		May	July	Sept.	Nov.	Dec.
Temperature	1	15	18.7	15.4	13.6	13
	2	17.7	19.1	15.1	13.2	13.1
	8	12.8	17	15.8	11.6	11
Nitrate	1	250	242	26	63	60
	2	525	521	189	60	56
	8	545	543	376	73	62
Dissolved Oxygen	1	8	8	8.1	8.7	8.5
	2	9.8	9.7	9.2	8.6	8.7
	8	8.3	8.2	8.5	8.9	9
Chlorophyll a	1	1.67	1.7	1.76	1.85	1.83
	2	1.87	2.05	2.07	2.11	2.13
	8	0.49	0.51	0.53	0.53	0.54
CBOD	1	2.09	2.5	2.56	2.93	2.98
	2	2.1	2.42	2.68	2.7	2.6
	8	2.14	2.4	2.7	2.8	2.8
Ammonium	1	220	231	316.7	337	340
	2	180	195	243	303	304
	8	196.9	196.9	200.5	213	304
Total Phosphorus	1	0.83	0.8	1	0.9	2.95
	2	41	40	38	18.9	16.8
	8	56	50	41	30.1	16.4
Total Kjeldahl	1	159	168	221	372	410
	2	177	181	199	380	400
	8	149	156	209	380	384

Models are approximate representations of reality; they cannot accurately describe natural systems, and there is no single accepted statistic or test that validates a model. As a result, a validation phase is performed on the model to help establish the appropriateness of the calibration and to determine whether the model created during calibration has a true representation of cause and effect connections. One of the most common statistical tools used for calibrating the simulation model is R-squared R^2 also known as a goodness-of-fit measure for linear regression models, the equation:

$$R^2 = 1 - \frac{RSS}{TSS} \quad (\text{Eq. 18})$$

RSS= the sum of squared of residuals and TSS= the total sum of squares and it is a statistical metric that quantifies the proportion of the variation explained by an independent variable or variables in a regression model for dependent variables, in Table 3.2 the R^2 between simulated results and field measurements at segments 1, 2, and 8 for the state variables: temperature, nitrate, dissolved oxygen, chlorophyll a, CBOD, ammonium, total phosphorus, and total kjeldahl, the R^2 ranged in Table 3.2, $0.86 \leq R^2 \leq 1$ and according to [78] if the coefficient of determination is $0.75 \leq R^2 \leq 1$ the performance rating is known to be very good. The second statistical test is relative error RE, which is used as a measure of precision, RE is the ratio of the absolute error of a measurement to the measurement being taken, in other words, this type of error is relative to the size of the item being measured, RE is expressed as a percentage and has no units

Table 3.2 Calibration of model result for state variables at Segments 1, 2, and 8

No	State Variable	Seg. No.	R ²	Relative error RE	Root mean square error RMSE	Mean absolute % error, MAPE
1	Temperature	1	0.93	34%	4.3	<88
		2	0.96	32%	4.1	<72
		8	0.91	9%	2.5	<40
2	Nitrate	1	0.97	186%	35.4	<86
		2	1	152%	129	<33
		8	0.96	178%	80	<23
3	Dissolved Oxygen	1	0.86	17%	1.7	<22
		2	0.97	10%	1.2	<20
		8	0.93	7%	0.9	<15
4	Chlorophy ll a	1	0.97	8%	0.4	<31
		2	0.98	18%	0.6	<24
		8	0.92	70%	1.4	<66
5	CBOD	1	0.97	7%	0.24	<12
		2	0.96	8%	0.2	<12
		8	0.98	26%	0.7	<40
6	Ammonium	1	0.98	4%	113.2	<30
		2	0.96	5%	13.9	<15
		8	1	11%	48.6	<24
7	Total Phosphorus	1	0.99	45%	0.3	<80
		2	0.93	42%	19.3	<58
		8	0.95	30%	16	<40
8	Total Kjeldahl	1	0.98	8%	47.6	<18
		2	0.88	26%	112.6	<63
		8	0.99	4%	11.3	<11

$$RE = \{(|\text{Actual value from site} - \text{value from model}|) / \text{actual value from site}\} \text{ (Eq.19)}$$

The latter in eq.19, on the other hand, should be handled with caution if the observed value approaches zero, the objective function is inflated by assigning a high weight to the linked observations, however, there is no upper limit on a “percent error” there is only the necessary human judgment on whether the data is acceptable or not, the values of RE in Table 3.2 are acceptable [79] except for nitrate which has a higher RE percentage than the other state variables.

So another test was performed only on these data of nitrate to ensure the model results are performing well since the R^2 for nitrate results are acceptable [78]. The Nash–Sutcliffe model efficiency coefficient NSE is used to assess the predictive skill of hydrological models- for nitrate, it is defined as [80,81]:

$$NSE=1-\frac{\sum_{t=1}^T(Q_0^t-Q_m^t)^2}{\sum_{t=1}^T(Q_0^t-\bar{Q}_0)^2} \quad (\text{Eq.20})$$

\bar{Q}_0 is the mean of observed discharges, and Q_m^t is modeled discharge and Q_0^t is observed discharge at time t , the Nash–Sutcliffe efficiency is calculated as one minus the ratio of the error variance of the modeled time series divided by the variance of the observed time series, this indicator can be used to describe the predictive accuracy of other models as long as there is observed data to compare the model results to [80]. The results of NSE Nash–Sutcliffe efficiency can be used to quantitatively describe the accuracy of model outputs with observed data, for the state variable of nitrate were 0.9, 0.84, and 0.92 for segment 1, segment 2, and segment 8, respectively, since they are ≥ 0.8 the results are acceptable [81].

According to Table 3.2, the result for Root mean square error RMSE is presented for the state variable, RMSE value indicates how concentrated the data is around the line of best fit, to validate experimental data, root means the square error is often utilized in climatology, forecasting, and regression analysis because it is scale-dependent, it can only be used to evaluate prediction errors of various models or model configurations for a single variable, not between variables, the equation used :

$$RMSE=\sqrt{\frac{\sum_{i=1}^n (\tilde{y}_i-y_i)^2}{(n)}} \quad (\text{Eq.21})$$

$\tilde{y}_1, \tilde{y}_2, \dots, \tilde{y}_n$ are the predicted values. y_1, y_2, \dots, y_n are the observed values. And (n) is the number of observations. RMSE is important since it is in the same units as the response variable and may be understood as the standard deviation of the unexplained variance, lower RMSE values imply a better match, and the root means square error RMSE is a good indication of how correctly the model predicts the response, and it is the most essential fit criteria if the model's primary objective is prediction [79].

The effect of localized significant mistakes even in limited geographical, temporal, or parameter areas is an immediately recognizable drawback of the RMSE for deterministic applications; the mean absolute error is frequently employed to lessen the effects of a few large errors as presented in the last column of Table 3.2.

MAPE is the Mean Absolute Percentage Error between measured and model results, it is a metric for determining how accurate a forecasting system it calculates the average absolute percent inaccuracy for each period minus actual values divided by actual values to compute this accuracy as a percentage, using the following [82]:

$$\text{MAPE} = \frac{1}{n} \sum_{t=1}^n \left| \frac{A_t - F_t}{A_t} \right| \quad (\text{Eq.22})$$

A_t is the actual value, F_t are the predicted values and (n) is the number of fitted points, although the idea of MAPE appears to be extremely easy and persuasive, it has significant limitations in actual application, and there is much research work on flaws and misleading findings from it, that MAPE is subject to overstating error because of the presence of extreme outliers or very large percentage errors has long been known, but compared with previous researches our results are acceptable [82], [83] and [84].

3.2 Sediment Oxygen demand (SOD)

Sediment oxygen demand (SOD) is thought to be an important factor influencing dissolved oxygen (DO) concentrations and has become an essential component in modeling DO in surface water bodies, several physical-chemical processes in the aquatic environment can influence the transit and interaction of nutrients, phytoplankton, carbonaceous material, and DO, SOD rates reported in natural habitats are caused by soluble organic compounds in the water column obtained from naturally occurring sediments containing aquatic plants, animals, and detritus [68]. Although the SOD value has the potential to have a significant impact on the overall oxygen demand in a water system, no widely acknowledged standard or standardized process for measuring SOD has been agreed upon [28], however, since there is no available data for sediment oxygen demand SOD at the site, and we need to ensure that our model result is representative for SOD, therefore a novel approach is adopted, which is based on the work of Sharma [74]. The results are presented in Table 3.3 for segments 1, 2, and 8 respectively Figure 3.1

The WASP model sediment diagenesis model replicates flow rates in geographically and temporally changing amounts that are governed by the quantity of organic material in the sediment, based on the rate of decomposition of particulate organic carbonaceous and nitrogenous material in the sediment, it also estimates sediment oxygen demand and fluxes of aqueous methane, gaseous methane, ammonia, and gaseous nitrogen at the sediment-water interface. Our model work keeps track of the amount of particulate organic material that settles out of the water column and accumulates in the sediment, as well as the amount of organic material in the sediment that is consumed by the decomposition process, to maintain a mass balance on reactive carbonaceous and nitrogenous material in the sediment, as a result, the WASP sediment oxygen demand component is intended to automatically adjust to variations in input loads.

Table 3.3 SOD results from applying equation and SOD from the model at segments 1, 2 and 8

Segment 1	Month	DOC-Model	SOD-from Equation	SOD-from Model
	July	0.94	0.11	0.52
	August	0.96	0.11	0.42
	September	1.18	0.12	0.4
	October	1.24	0.12	0.39
	November	1.24	0.12	0.39
Segment 2	Month	DOC-Model	SOD-from Equation	SOD-from Model
	July	1.1	0.12	0.5
	August	1.1	0.12	0.46
	September	1.26	0.12	0.39
	October	1.24	0.12	0.39
	November	1.24	0.12	0.38
Segment 8	Month	DOC-Model	SOD-from Equation	SOD-from Model
	July	1	0.11	0.48
	August	1.09	0.12	0.47
	September	1.17	0.12	0.41
	October	1.22	0.12	0.38
	November	1.26	0.12	0.36

However, the next step would be the calibration of results using R^2 and RE to compare the SOD model and SOD from the equation with results presented in Table 3.4 and Figure 3.1

Table 3.4 Calibration result of SOD at segments 1, 2 and 8

Diagenesis Model	Segment	R ²	RE relative error
SOD	Segment 1	0.63	0.73
	Segment 2	0.91	0.71
	Segment 8	0.94	0.61

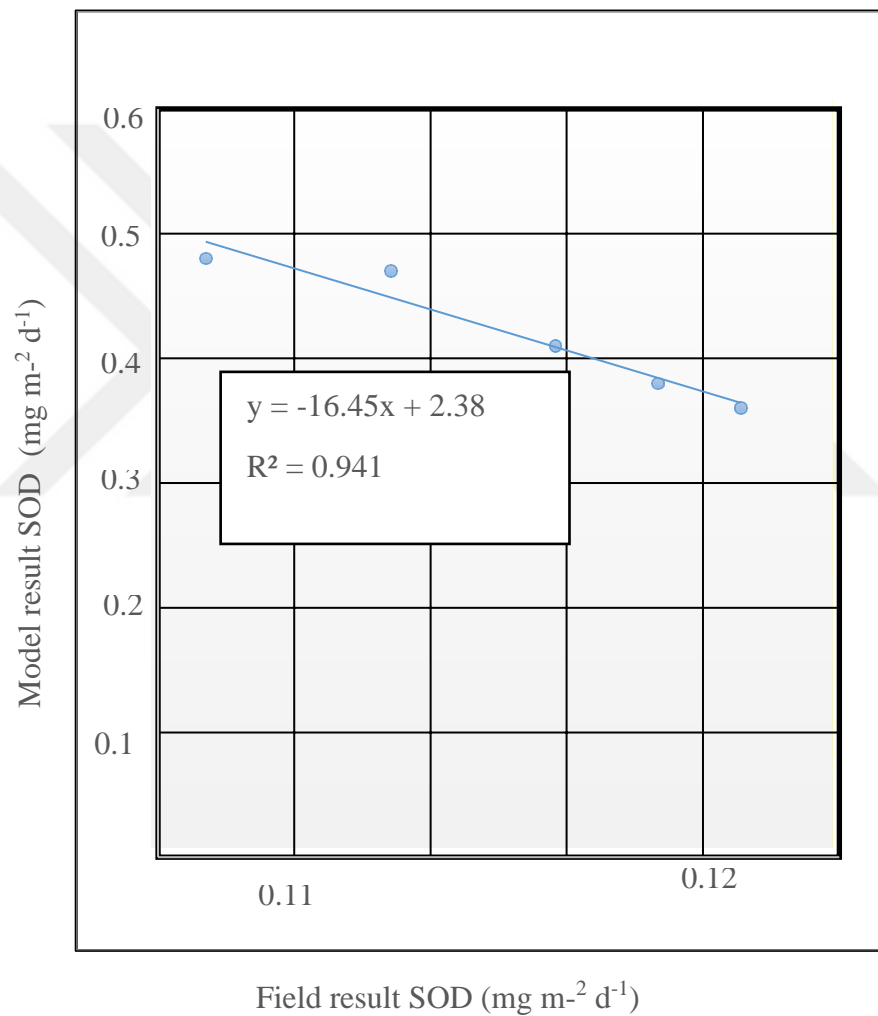


Figure 3.1 Statistical test R² for SOD model and SOD equation. R² =0.94 calibration result for segment 8

3.3 Internal nutrient loading

Cultural eutrophication is the process by which nitrogen and phosphorus from anthropogenic sources enter the environment and increase primary production. This symptom in freshwater systems includes changes in algal community structure, food web shifts, hazardous algal blooms, and oxygen decreases due to aerobic decomposition. These conditions not only reduce water quality for biota but also cause financial losses in property values and recreation costs. However, as nutrients enter a lake or reservoir through erosion and runoff, they accumulate in the sediment, creating the possibility of an internal load that might be discharged back into the water column under different environmental conditions. Historically, eutrophication treatment has focused on reducing external nutrient inputs. be discharged back into the water column under varying environmental conditions.

Anoxia can affect the amount of nitrogen in lakes and reservoirs because nitrate reduction is an anoxic, bacterial-mediated process that happens in sediments and converts nitrate to ammonium. This activity is important for the environment because it supplies nitrogen in a dissolved form that is redox-mediated in phosphate-binding iron hydroxides, which release P via the redox-mediated iron reduction in. [38]. Denitrification is similarly an anoxic, bacterially driven process, but it serves as a nitrogen sink by converting nitrate to nitrogen gas, nutrients released from sediments under anoxic circumstances can change Nutrient ratios and concentrations in the water column TN:TP Changes in the TN:TP ratios, which can then be used to determine which nutrient is limiting in a system at any given moment, can indicate changes in nitrogen and/or phosphorus availability, and therefore the nutritional status of phytoplankton, if they reach the epilimnion via diffusion and/or water column mixing. Additionally, when TN:TP ratios are low, cyanobacteria can dominate because they can fix atmospheric nitrogen and outcompete other species when nitrous, which can alter the total phosphorus budgets and release rate estimations. Furthermore, the chemical makeup of the sediment, such as iron and iron: phosphorus ratios, as well as PH, has been demonstrated to impact sediment nutrient release rates, as a result, greater knowledge of these parameters, in conjunction with observed release rates, will be critical to completely comprehend the entire significance of sediment phosphorus

release [38]. The model also simulated other phenomena occurring in sediment that contributed to increased levels of SOD at segment 8 and an overall dissolved oxygen deficiency in the water column. Internal phosphorus from anoxic sediments affected water column nutrient concentrations and ratios of TN:TP at the reservoir and the PO₄ flux to the water column in (mg P/m²-day) would increase the internal loading release and thus decrease DO at the reservoir, the ratio of TN:TP is based on the model result at Table 3.5

Table 3.5 ratio of total nitrogen to total phosphorus simulated by the model at segment 8

Month	TN Simulated by model	TP Simulated by model	TN:TP ratio	interpreting the result of the TN:TP ratio
July	156	50	3	Ratio<9 N limited
August	209	41	5	Ratio<9 N limited
September	380	30.1	13	<9 Ratio <22
November	384	16.4	23	Ratio> 22 P limited

Anoxic processes appeared to alter nitrogen in the reservoir, which may have influenced nutrient restriction further, in the hypolimnion, both total nitrogen and nitrate levels declined but the general declining trend in total nitrogen concentrations shows that hypolimnetic processes were serving as a sink for nitrogen in the system, and these processes, in conjunction with internal phosphorus release, aided in increasing the TN:TP ratio, as phosphorus is the limiting factor as it may be limited by a natural scarcity of the nutrient in the environment during stratification and mixing in the reservoir.

3.4 The process of calibrating our model

Once the model was executed it was subjected to a thorough calibration before its used for determining the sediment oxygen demand, with this intention, the results obtained from a series of calibration runs were compared with prescribed sets of field measurements, and the results of calibration were then checked using statistical tools as presented in Table 3.1 of model result starting from May to December of

the year 2019 for the state variables: temperature, nitrate, dissolved oxygen, total phosphorus, chlorophyll a, total kjeldahl, BOD, and ammonium at segments 1, 2, and 8. The results are then calibrated in Table 3.2 by applying the statistical analysis methods to check the accuracy of model results with actual measured data from the site, the first method used is R squared R^2 which is a statistical measure of how close the data are to the fitted regression line between measured field data and the model result, from Table 3.1 our range for the state variables is between 0.86 and 1.0 according to Moriasi [87], higher values indicate less error variance and are acceptable. In Table 3.2 RMSE is calculated for the simulated results and RMSE is defined as the root mean square error of approximation and its absolute measure of fit, the range for RMSE is from 0.2 to 129 according to previous research the sensitivity of the RMSE to outliers is the most common concern with its use, RMSE has no clear interpretation [88], [89], [90], and [91], therefore for our model calibration, we will not depend on RMSE techniques, the column of mean absolute percentage error results to be a very large value even though the model appears to fit the data well, this is because it divides the absolute error by the actual data when the values, which are at times closer to 0, can greatly inflate the result of RMSE. The last test we performed was the relative error RE between simulated and measured data, RE is all less than 1 which indicates good results according to Hazewikel [88] except for the nitrate which is 1.86, 1.52, and 1.78 for segments 1, 2, and 8, respectively, so another test was performed only on these data of nitrate to ensure the model results are performing well since the R^2 for nitrate results are high, the results of NSE for the state variable of nitrate were 0.9, 0.84, and 0.92 for segment 1, segment 2, and segment 8 respectively, according to [87] where $NSE > 0.75$ is found to be acceptable. The simulation model we created using WASP8 represents the actual case of the Kurtboğazı reservoir, according to the results of calibration to our model. The next step would be to use the quality model to achieve the goal of this research, which is the investigation of sediment oxygen demand and the rate at which dissolved oxygen is removed from the water column in surface water bodies due to the decomposition of organic matter in the bottom sediments., this involves using Sharma's equation [74] by applying the total organic carbon from the sediment diagenesis model and applying to equation (17) to obtain SOD, which is regarded

as the SOD field, and calibrating the results of the diagenesis simulation model with the SOD field that exhibits high values for R^2 as follows: the R^2 for segment 1 is 0.63, for segment 2 it is 0.91, and for segment 8 it is 0.94. The reason that R^2 is much lower in segment 1 than in the other locations could be because segment 1 is the inlet point arriving from the İnceğiz tunnel which derives water from the Eğrekkaya dam to Kurtboğazı reservoir [48] therefore, the occurrence of unaccounted nutrients could be found that are entering the reservoir and causing the different SOD values and according to Van [87] values of R^2 greater than 0.5 are considered to be acceptable.

Stratification is the process by which reservoir waters are separated into stable strata of varying densities, deep hypolimnetic water is colder and frequently low in oxygen due to consumption from decaying organic matter exceeding replenishment from the surface, hypoxia also causes the release of sediment-bound nutrients as well as decreased redox-active molecules like hydrogen sulfide and ammonia, which can reach lethal levels, because of heterotrophic consumption and a lack of replenishment from oxic top layers, stratification tends to deoxygenate deep reservoir water, in addition to the immediate impact of hypoxic reservoir water when released downstream, anoxic bottom waters initiate a series of anaerobic redox reactions inside reservoir sediments that change water quality further, as a result, anoxia can cause indirect chemical changes and related ecological effects, in the summer because stratification is the process of forming thermal layers in a reservoir or lake, the water temperatures in the upper layer get warmer while the bottom layer becomes cooler, this will result in a temperature differential phenomenon ending in variances in densities between the top and lower layers, which leads to thermal stratification [70] and [76], this was successfully simulated by our model as presented in Figure 3.2, according to previous researchers accomplished by [15], [35], [36], [58], and [60] from the simulation result of our model presented in Figure 3.3, it is concluded that our result following previous research findings, with increasing total phosphorus and peak maximum value of total phosphorus; water temperature; nitrate, and dissolved oxygen corresponded to the highest SOD value.

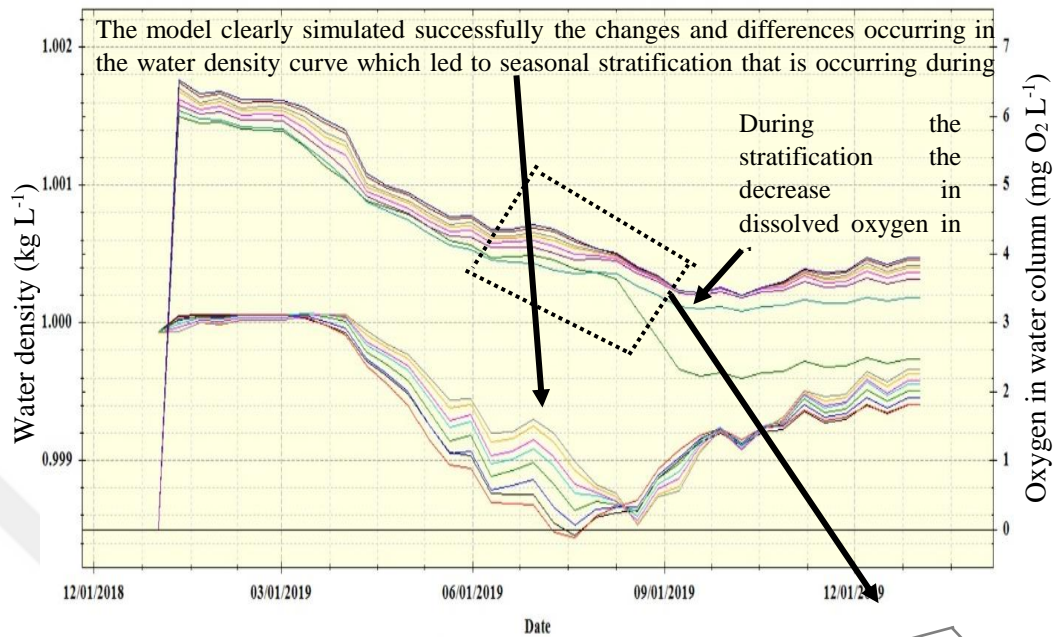
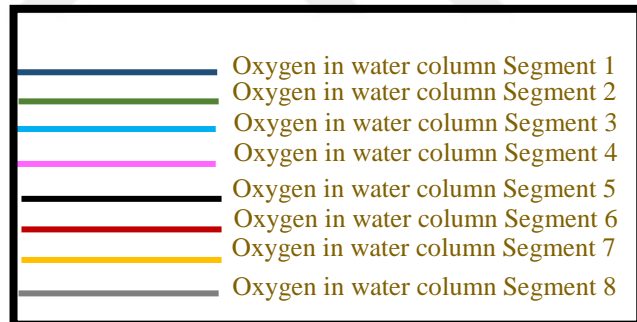


Figure 3.2 Water density & dissolved oxygen level in the water column along with the dissolved oxygen for all 8 segments



There is a correlation of between SOD and TP up to 98% which indicate that an increase in nutrients cause an increase in oxygen consumption and eventually increase SOD.

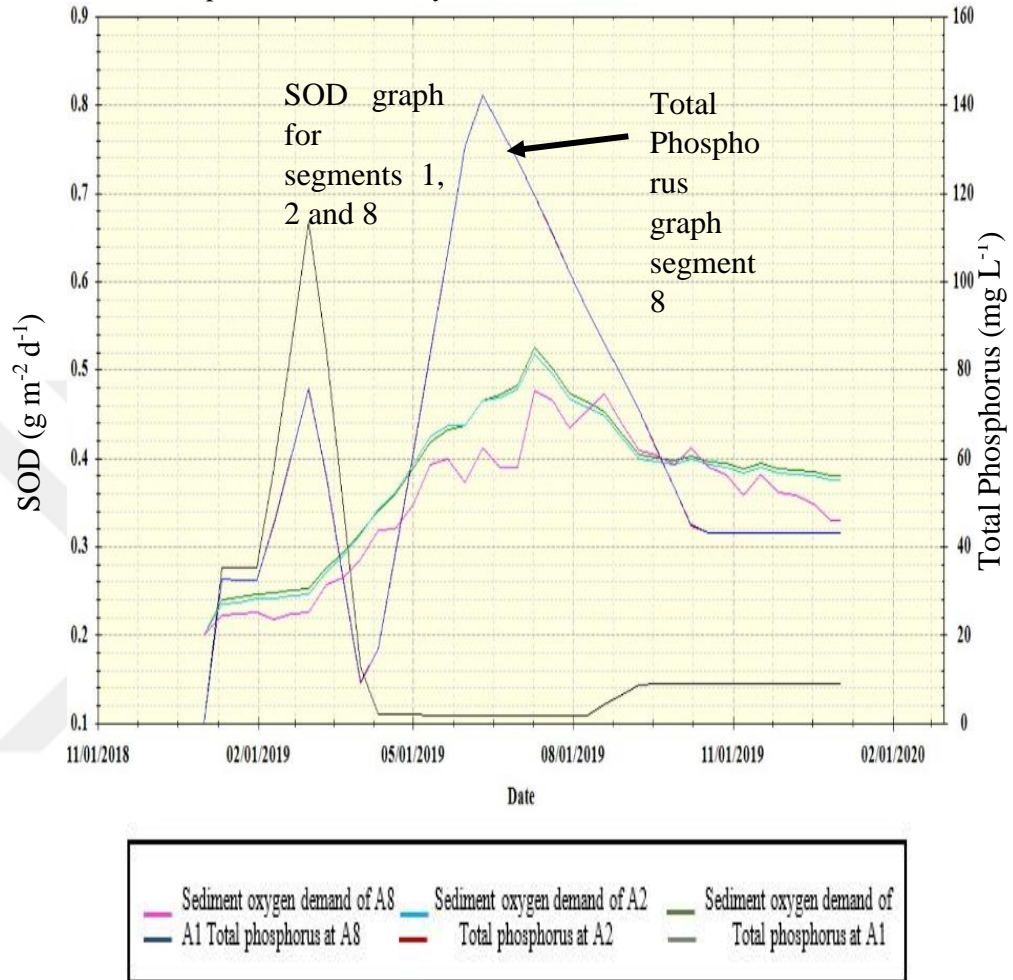


Figure 3.3 Influence of total phosphorus on sediment oxygen demand according to our model simulation result.

There is a correlation between SOD and TP which indicate that an increase in nutrients causes algal bloom and eventually an increase in SOD, according to model results the graph correlation between SOD and phosphorus is up to 93% which indicates that an increase in nutrients increases the consumption of oxygen that leads to an increase in SOD.

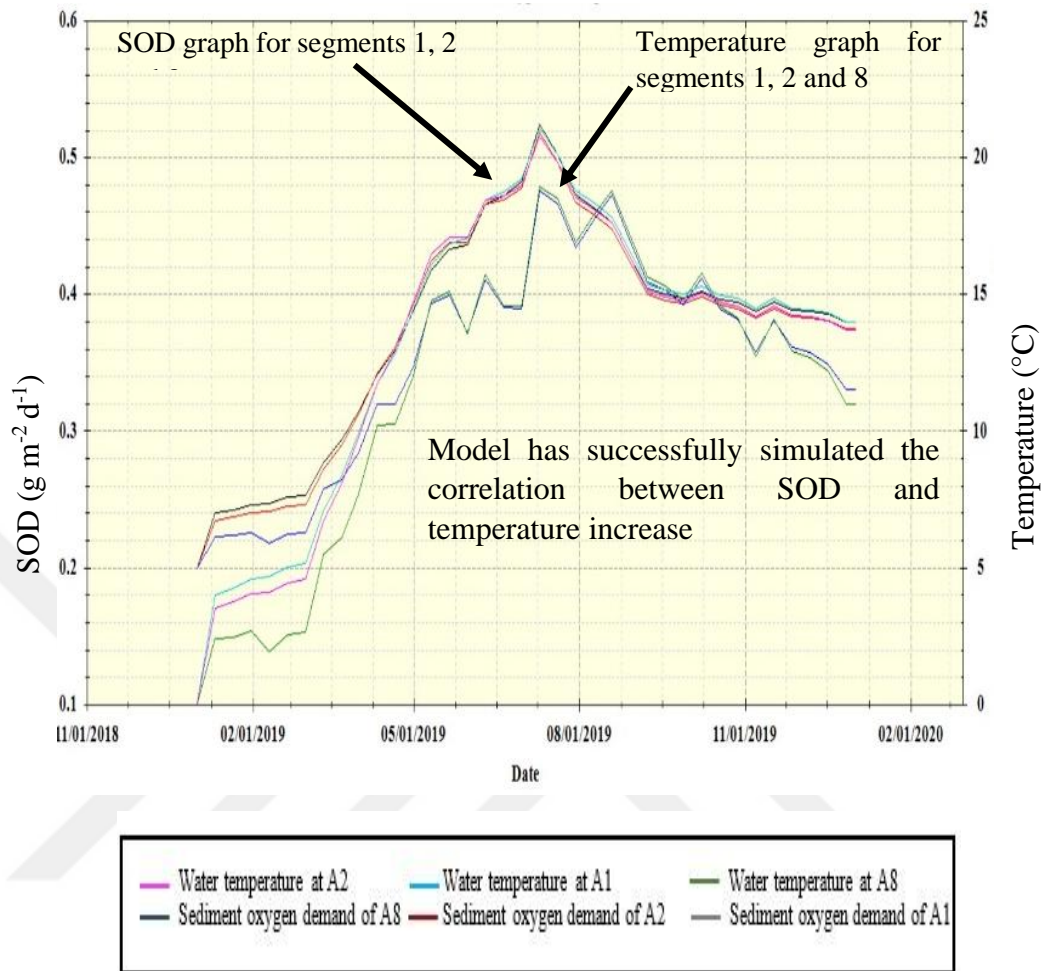


Figure 3.4 Temperature variation and its effect on Segments 1, 2, and 8 for the simulated system.

The model has successfully simulated the correlation between SOD and temperature as cold water can hold more dissolved oxygen than warm water, which eventually increases the SOD levels.

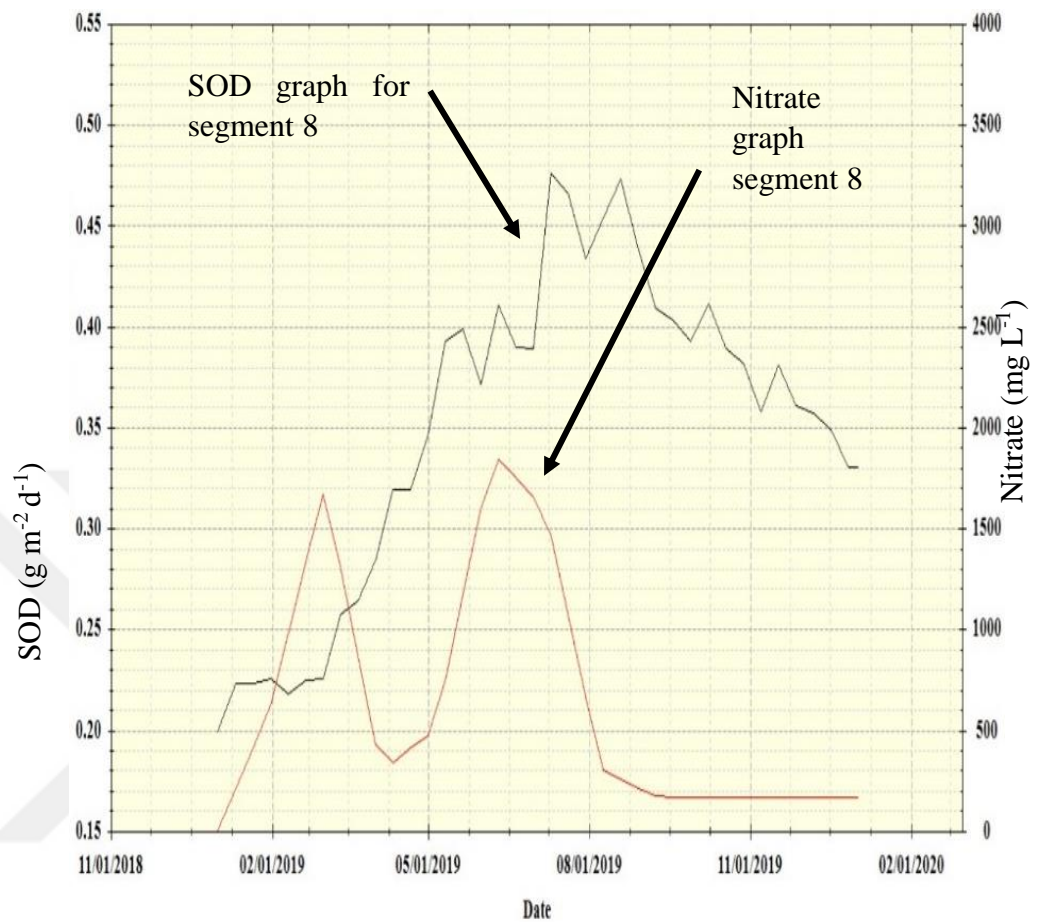
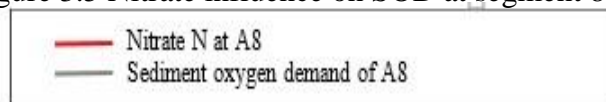


Figure 3.5 Nitrate influence on SOD at segment 8



There is a correlation between SOD and Nitrate up to 93% which indicates that an increase in nutrients increases the phytoplankton and algal blooms which increase the consumption of oxygen leading to an increase in SOD for segment 8 in the model.

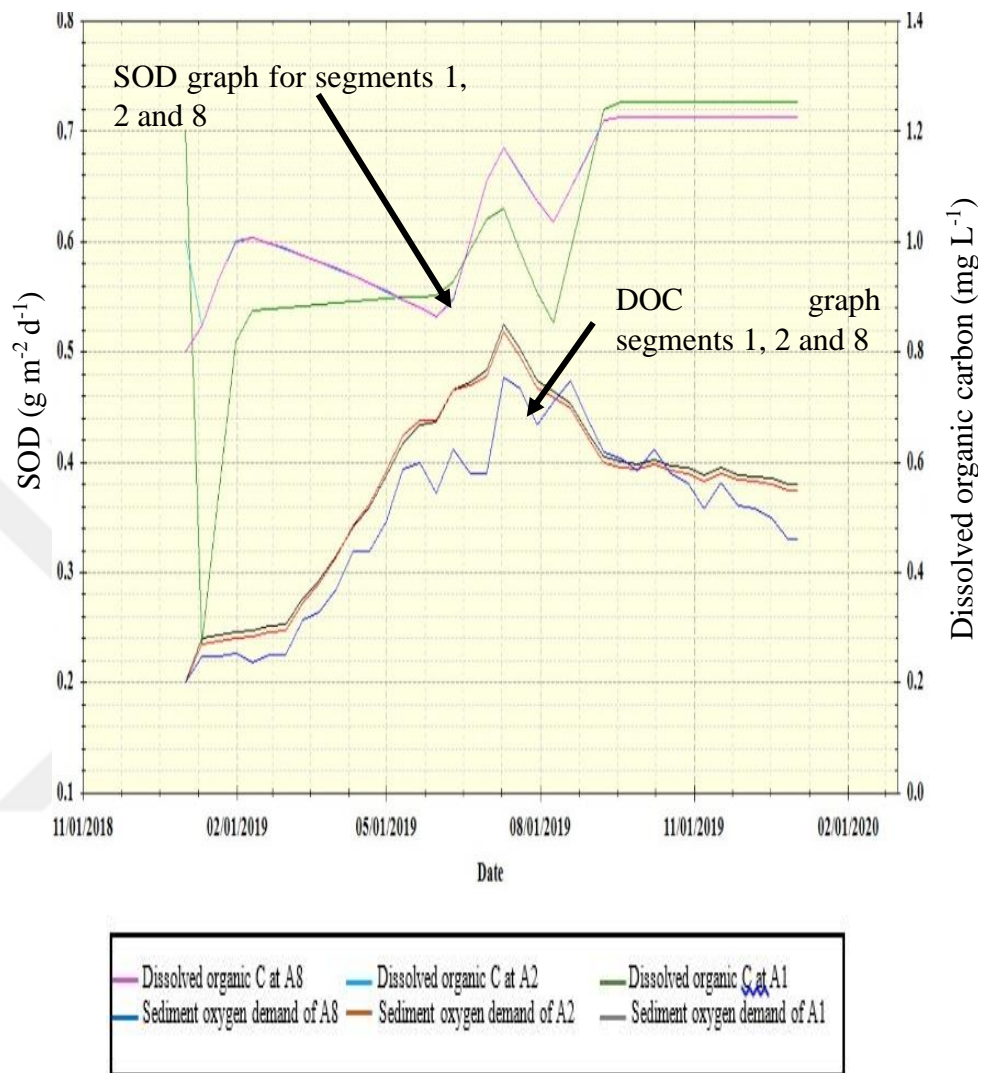


Figure 3.6 the effect of dissolved organic carbon on SOD at segments 1, 2, and 8 for the simulation model

The organic waste is decomposed by bacteria that eventually lead to the removal of oxygen removal and an increase in SOD, the model successfully calculated a correlation of up to 95% between SOD and dissolved organic carbon, marked by the development of anoxia condition our results are in accordance with Lantrip [72].

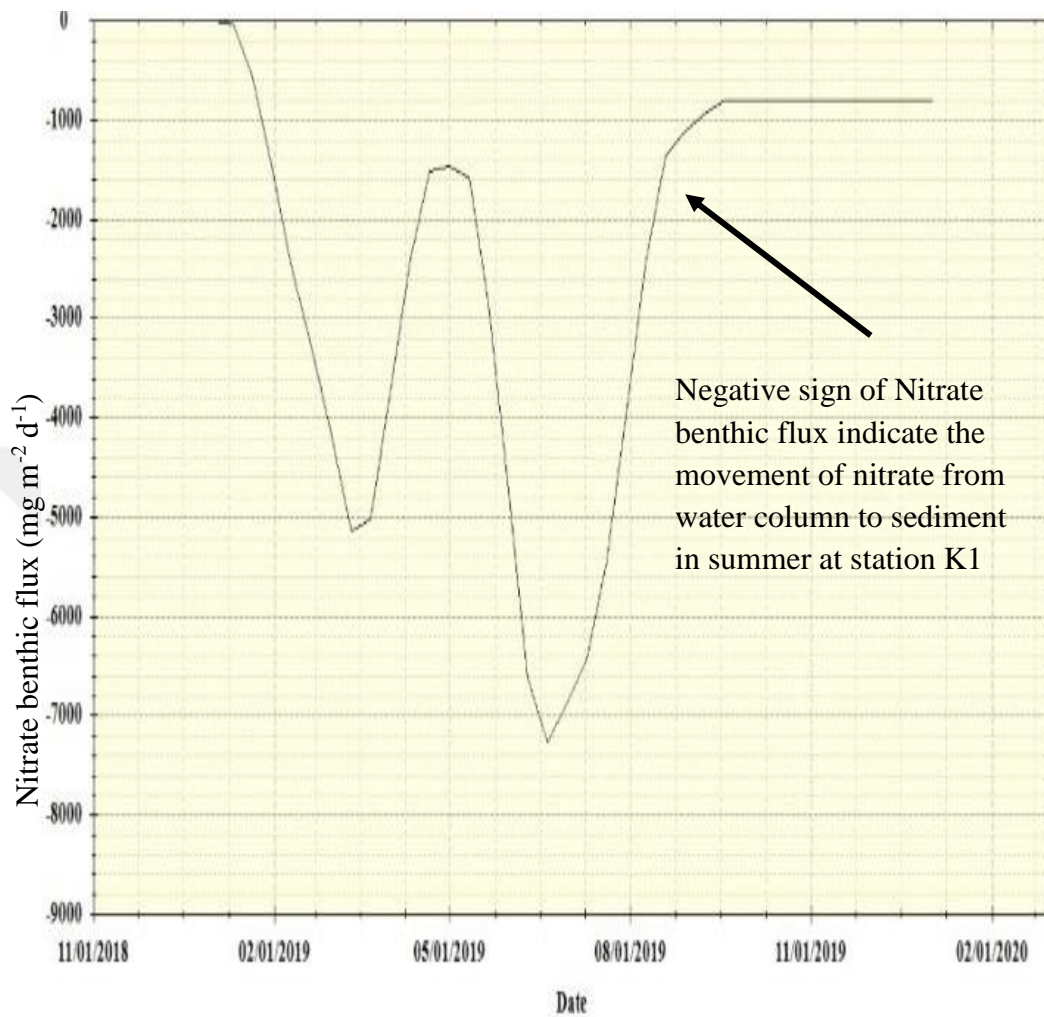


Figure 3.7 Simulation of nitrate benthic flux at segment 8

The model simulated as shown the effects of anoxic conditions on the SOD at segment 8 in the model, Figure3.7 Graph of nitrate benthic flux and the negative sign indicate the movement of nitrate from the water column to sediment in summer at segment 8

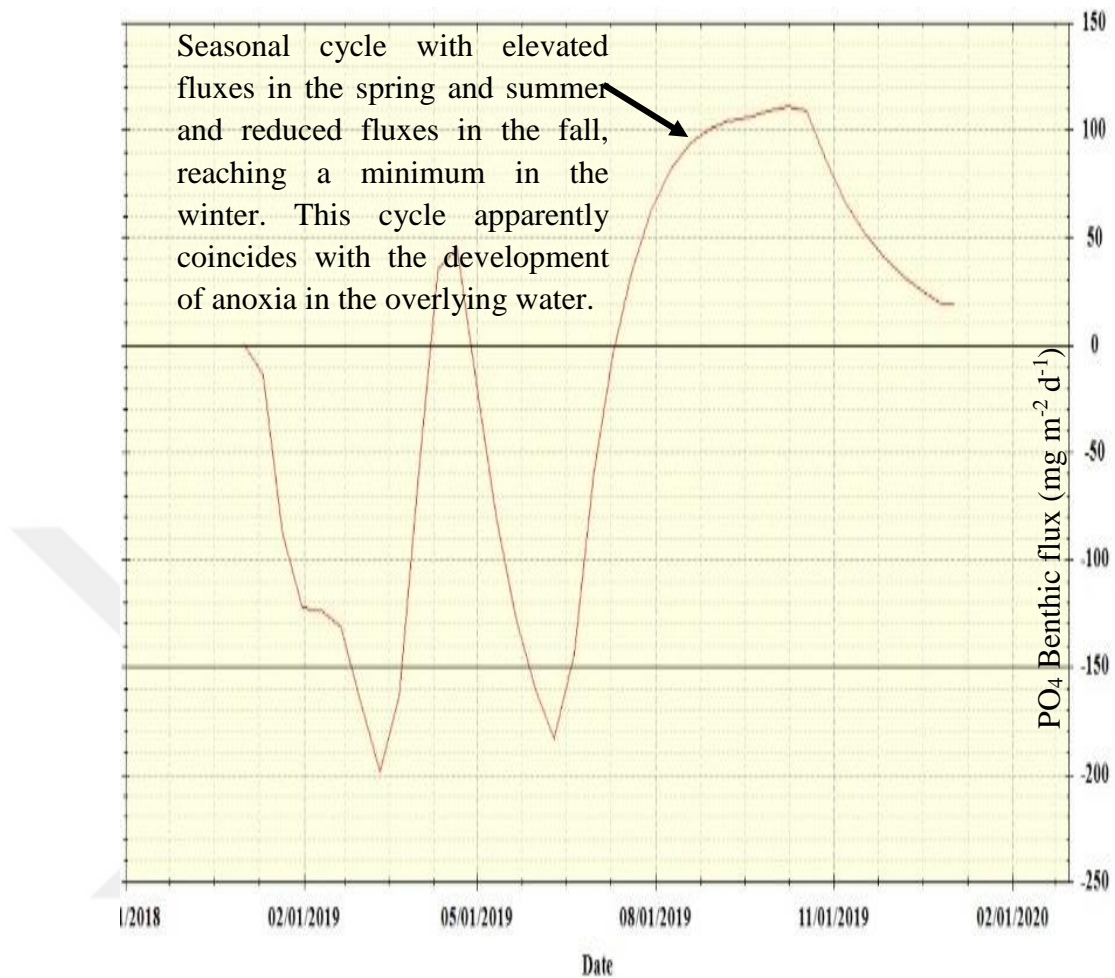


Figure 3.8 Simulation result of model for the PO₄ benthic flux

The PO₄ benthic flux graph which displays a seasonal cycle with elevated fluxes in the spring and summer and reduced fluxes in the fall, reaching a minimum in the winter, this cycle coincides with the development of anoxia in the overlying water of seg. 8.

Figure 3.9 below displays the dissolved inorganic phosphorus benthic flux with increased movement of available phosphorus from sediment to the water column during anoxic conditions specifically rise at summer and ammonium benthic flux variability observed in spring and summer, with a general reduction in flux to sediments in summer that reflects a temperature or biological community dependency

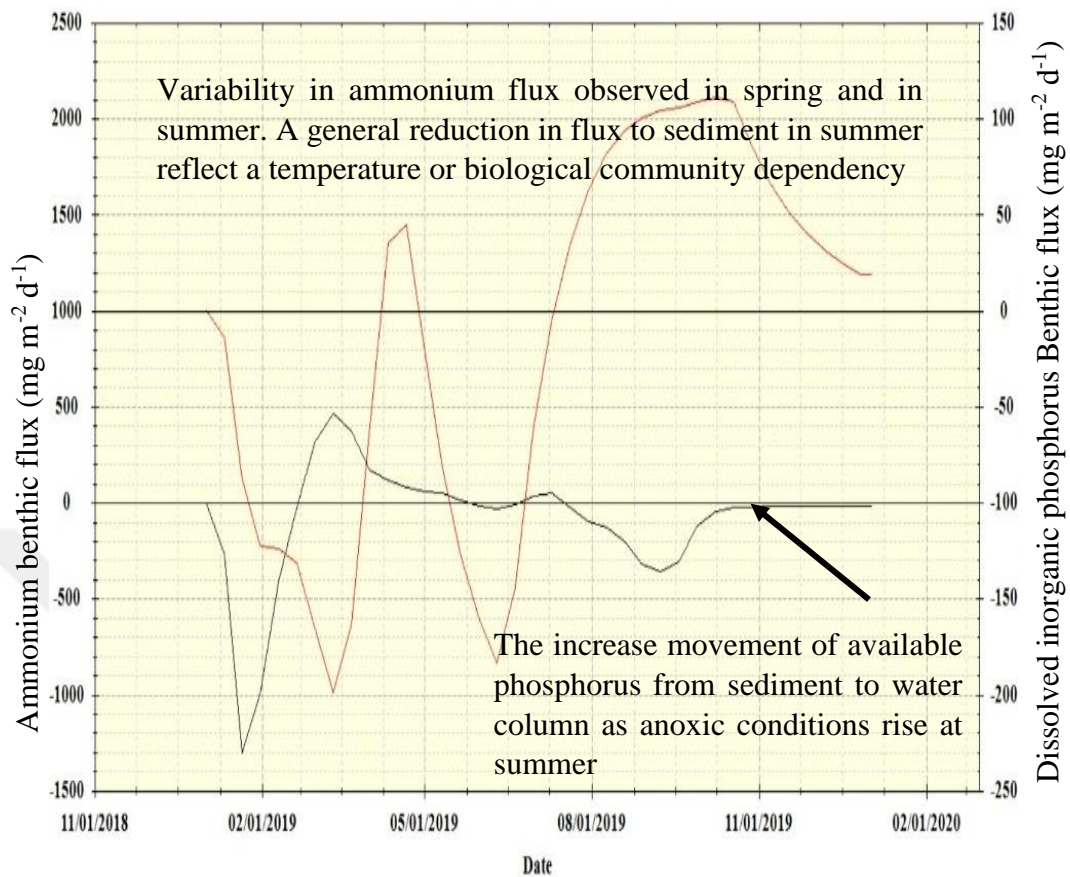


Figure 3.9 displays the dissolved inorganic phosphorus benthic flux with increased movement of inorganic phosphorus

Nutrient flux rates from the sediment represent the net result of various microbiological, chemical, and hydrodynamic processes, this cycle coincides with the development of anoxia in the overlying water, phosphorus release involves the development of anoxia in the water column, resulting in the creation of reducing conditions in the sediments, with associated changes in the iron-phosphorus complexes, in an oxidizing environment, the iron which is in insoluble ferrous form, the formation of iron in the soluble ferric form, with the release of bound phosphorus this a rise in total phosphorus and TN:TP ratios, were highly associated with anoxic depth positive correlation negative correlation, using data from the mixing period only resulted in greater coefficients of determination for TP and TN:TP, suggesting

that late-season epilimnetic total phosphorus was impacted by internal phosphorus load it was responsible for the observed reduction in epilimnetic TN:TP ratios, as a result, the internal phosphorus load can have a significant impact on nutrient concentrations and ratios in the epilimnion of eutrophic reservoirs, previous research has also demonstrated that internal phosphorus loading can play a significant impact in late season algal blooms [38, 85, 86].

Internal phosphorus from anoxic sediments affected water column nutrient concentrations and ratios of TN:TP at reservoirs according to Nikolai [38], Guilford [92], and Downing [93], when the resulting ratio for nitrogen to phosphorus TN:TP ratio > 22 indicates phosphorus limitation or decrease in phosphorus nutrient if TN:TP ratio < 9 indicates nitrogen limitation or decrease of nitrogen nutrient and in the case of nutrient ratio $9 < \text{TN:TP ratio} < 22$ indicating P and N co limitation both nutrients P and N are limited. As the thermocline layer of water is more often found in a large body of water, where the temperature gradient is greater than that of the warmer layer above and the colder layer below decreases in the late summer, according to the model result in Table 3.5 the TN:TP ratio shift from N limited during the summer to P limited at the beginning of winter internal P can build up in the hypolimnion and help to lower TN:TP ratios and potentially create N limiting conditions in the epilimnion, previous studies have similarly shown that internal P loading can play an important role this result is in accordance with [38], [92], and [93]. Another indication from the result of the simulated model is by examining the denitrification flux from sediment, it is obvious from Figure 3.10, the increase of N_2 gas at the water column during the stratification phase explains the N limited for the TN:TP ratio during that time, the period of high denitrification and increase of N_2 gas occurring at anoxic phase and affecting the TN:TP ratio by causing nutrients to be N limited as shown in Table 3.5, as the thermocline eroded and hypolimnetic P mixed with the epilimnion, TN:TP ratios would fall, and the reservoir would possibly become N-limited.

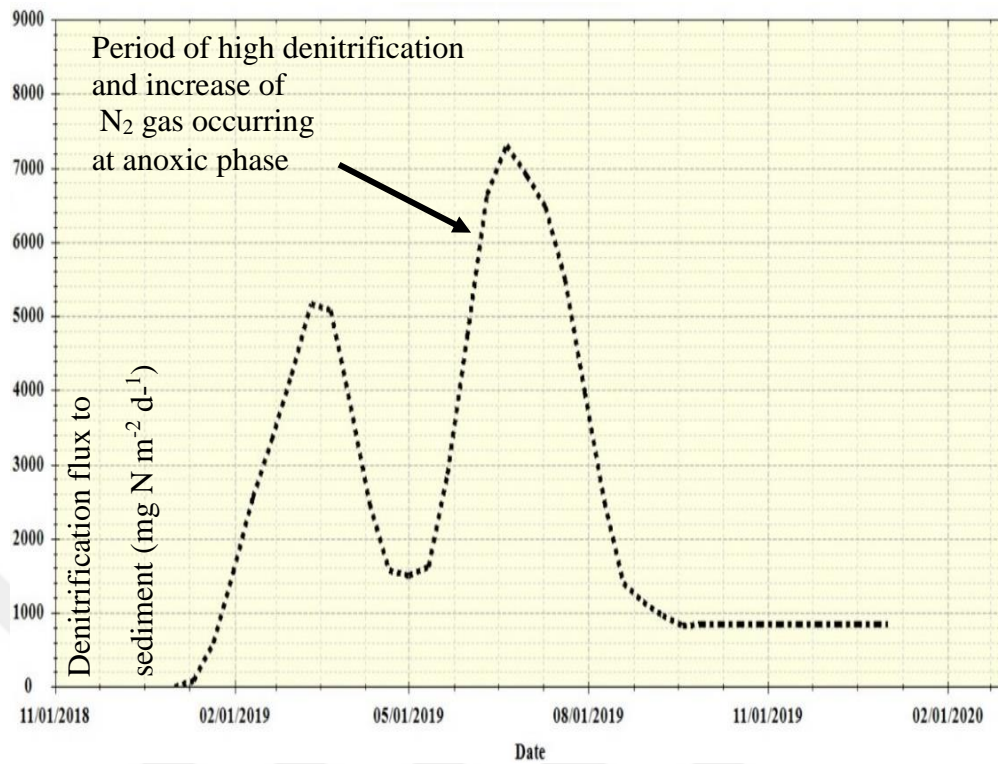


Figure 3.10 Denitrification flux at anoxic phase from sediment to Water column at segment 8

The thermocline began to erode before mid-August, and the overall trend was from P limitation or N and P co-limitation in early August to N limitation in September.

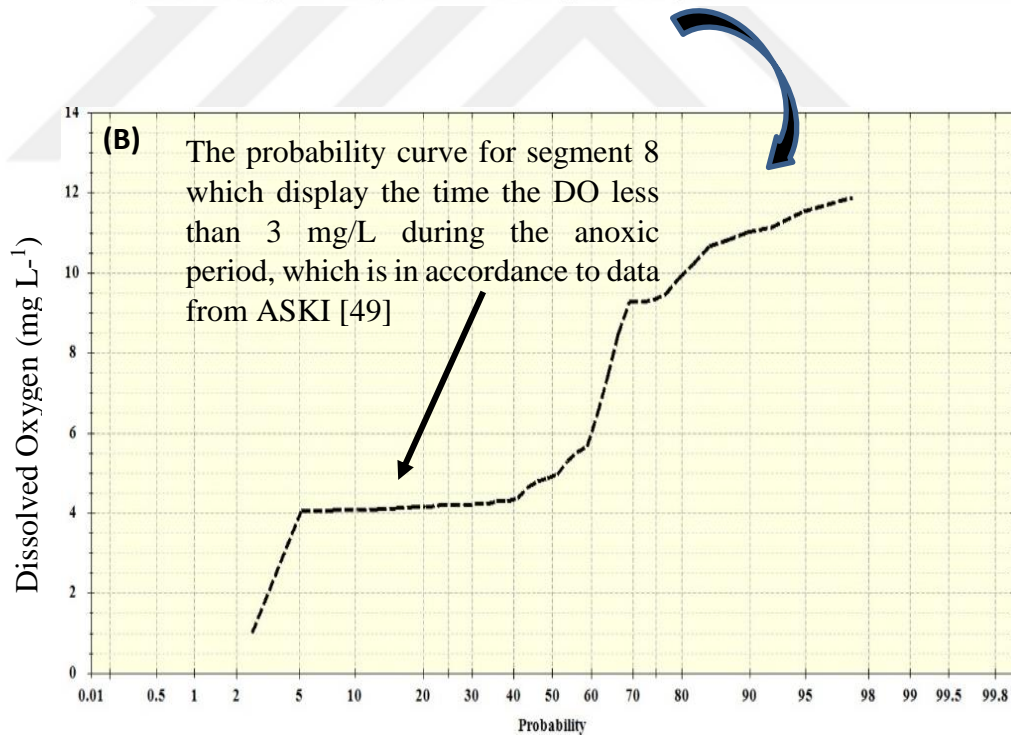
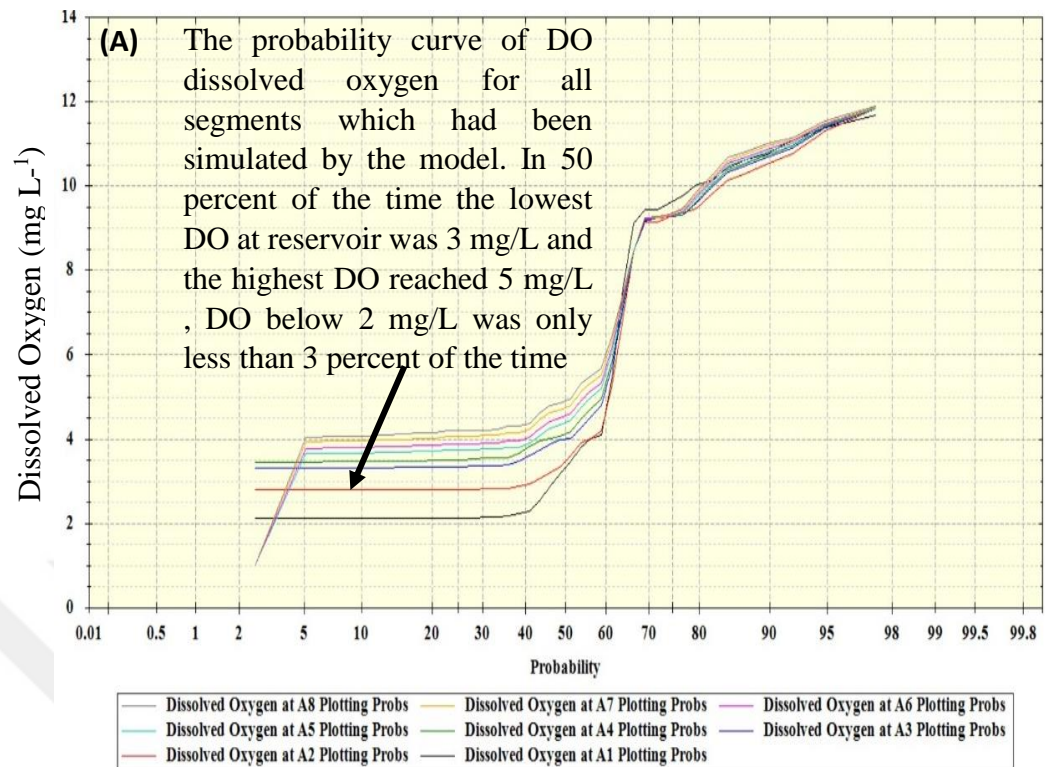


Figure 3.11 Probability curve and simulated model result for dissolved oxygen at the model segments

in Figure 3.11 (A) the probability graph shows that 50 percent of the time the lowest DO at the reservoir was 3 mg/L and the highest DO reach 5 mg/L, DO below 2 mg/L

was only less than 3 percent of the time. Figure 3.11 (B) The probability curve for segment 8 displays the time the DO is less than 3 mg/L during the anoxic period, which is in accordance with [49].

3.5 Model Validation

Calibration always trains the model for certain hydrological conditions, which are those resembled by the observed data, when used in so-called "out of sample settings," i.e., hydrological conditions that differ considerably from those referred to in calibration, the model may offer less desirable results in terms of what resulted from calibration, this is a key practical issue that may have a detrimental influence on the reliability of engineering design, because of the uncertainty that affects hydrological models, validation is always important in model simulation design. After calibration and before utilizing it in reality, we proposed a more extensive validation techniques, such as cross-validation applications, the word validation is often used in hydrology and environmental modeling to describe a technique for examining the performance of simulation and/or forecasting models, however, in the scientific environment the word validation has a broader definition that includes any method that aims to test a procedure's capacity to fulfill a certain scope, in other words, it's the degree needed for the model's intended purpose or application, and this is achieved through determining the representative output of our simulation model, this is achieved through tracing the intermediate results and comparing them with observed outcomes, and this method involves investigating the intermediate interaction between key variables in the system, in our case the dissolved oxygen and sediment oxygen demand is selected as it has a high influence on the overall system, by utilizing correlation coefficient we trace the correlation of SOD, DO, temperature, and chlorophyll a with other state variables and compare with the outcome, to assess the correlation Pearson's coefficient was used to measure validity as its correlation is widely used to validate the strength of an existing linear relationship between variables, through assessments of the linear relationship between quantitative variables [95]. The Pearson's correlation coefficient (ρ) is a way of determining if two variables have a close relationship, it is defined as the quotient of the covariance and the standard deviation of two variables, when ρ has been calculated the procedure

is designed so that the units of measurement do not affect the calculation. This allows the outcome result of the correlation coefficient to be comparable and not affected by the units of the variables used. Table 3.6 shows the outcomes of the calculations, the segment that was selected is segment 8 and the reason for this choice, is segment 8 represents the discharge point from the reservoir and according to site field data it is the critical point where the seasonal stratification and oxygen depletion occurs seasonally.

Table 3.6 Application of Pearson correlation to variables at segment 8

State variables	Sediment oxygen demand	Dissolved oxygen
Dissolved oxygen	0.77	
Temperature	0.89	0.79
Total Phosphorus	0.89	0.66
NO ₃	0.96	0.65
CBOD	-0.68	-0.70
Chlorophyll a	-0.70	-0.28
Sediment oxygen demand		0.77

The SOD has a high correlation with dissolved oxygen; temperature; total phosphorus; and nitrate this result is confirmed by many studies earlier that nutrients can increase eutrophication and later on an increase in SOD [23], [24], [25], [26] and [28], from table 3.6 dissolved oxygen is correlated with SOD for Pearson correlation = 0.77 and while the temperature correlation with SOD for Pearson correlation = 0.79 this is in accordance with [59], [68], [69], [72], and [74]. The dissolved oxygen has a moderate Pearson correlation with total phosphorus = 0.66 and Pearson correlation for nitrate = 0.65 this conclusion approved by earlier research [11], [13], [23], and [27]. As shown in Table 3.6 there is also a weak correlation between dissolved oxygen and chlorophyll a Pearson coefficient = -0.28 [94] and a high Pearson correlation between dissolved oxygen and sediment oxygen demand = 0.77 while the Pearson coefficient for CBOD and dissolved oxygen are negatively highly correlated = -0.70, which is often observed as the inverse strong relation between CBOD and dissolved oxygen [10, 41]. Our model was validated based on the concept of using Pearson's correlation coefficient and the state variables in the model, which in agreement with previous research.

CHAPTER 4

CONCLUSION

- The work adopted a sediment oxygen demand diagenesis model and a useful numerical tool for modeling a water body in both steady and erratic conditions. In general, the averaged model may estimate complex temporal relationships between state variables and situations in each of the physical processes that exist in real-life environments. A finite difference method was used to solve the resulting system of equations with a volume composition that encourages consistent and conservative performance solutions throughout all flow regimes. The diagenesis model includes the interactions of physical, chemical, and biochemical activities that result in significant changes to the sediment after deposition in the water body. The suggested model may correctly and reliably depict the reality of the interactions between hydrodynamics and quality thanks to calibration and validation, as a result, the integrated model can estimate water quality in a variety of settings, and this tool may be valuable to the entities delivering this service since it will allow them to decrease and accurately identify the placement of the quality measurement stations.
- The effect of anoxic conditions in summer on nitrate benthic flux causes the movement of this nutrient from the water column to sediments at station K1 or segment 8
- For the benthic flux regarding PO_4 at the seasonal cycle with elevated fluxes in the spring and summer and reduced fluxes in the fall, reaching a minimum in the winter, this cycle coincides with the development of anoxia in the overlying water.
- As for the effect of anoxic conditions on inorganic phosphorus benthic flux, it increases the movement of available phosphorus from sediment to the water column as anoxic conditions rise in summer and ammonium benthic flux variability is observed in spring and summer, a general, reduction in flux to sediment in summer reflects a temperature or biological community dependency.
- The anoxic phase is defined by the characteristics of the high denitrification process and the increase of N_2 gas production, these features have an effect on the

total nitrogen to total phosphorus ratio (TN: TP ratio) by causing nutrients to be limited, this was successfully simulated by the model.

- During the summer period, it was noted by the simulated model result to produce a positive correlation between sediment oxygen demand SOD and dissolved organic carbon [95], total phosphorus, temperature, and nitrate at segment 8 this phenomenon is manifested by the oxygen depletion and anoxic condition that occurred during that period, and all the model results are following field measurements.
- The probability curve of DO dissolved oxygen for all segments was stimulated by the model, in 50 % of the simulated time the lowest DO at the reservoir was 3 mg/L and the highest DO reach 5 mg/L, dissolved oxygen below 2 mg/L was only less than 3 % of the anoxic time.
- Our model was further validated using the Pearson correlation coefficient with results that were in accordance with previous research and model work.
- The developed model linked the oxygen depletion and the phenomena of sediment oxygen demand SOD, it can serve as a useful tool for water managers in the estimation of the parameters influencing the anoxic condition and benthic flux.

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APPENDIX A
WASP8 Model Input Criteria

Table A1 Surface horizontal distance and area
Between segments

Surface Horizontal		A=L*W	
From	To	Distance	Area
Boundary	A1	568	479960
A1	A2	1005	836552
A2	A3	889	679320
A3	A4	962	664428
A4	A5	1122	733992
A5	A6	1071	653004
A6	A7	991	679396
A7	A8	911	678299
A8	Boundary	379	739575

Table A2 Calculations for vertical exchanges

Vertical exchanges		A=W*D	
From	To	Distance	Area
A11	Boundary	16.7	14069.3
A22	Boundary	17.2	13994.4
A33	Boundary	16.2	11531.1
A44	Boundary	16.7	11155.5
A55	Boundary	17.2	10993.2
A66	Boundary	16.7	9457.2
A77	Boundary	17.7	13890.6
A88	Boundary	17.7	12090.3

A3 Calculations for surface exchanges

Surface Vertical		A=W*D	
From	To	Distance	Area
A1	A11	33.2	959920.0
A2	A22	34.2	713184.0
A3	A33	32.2	645456.0
A4	A44	33.2	683400.0
A5	A55	34.2	784584.0
A6	A66	33.2	521424.0
A7	A77	35.2	837368.0
A8	A88	35.2	519230.0

Calculations of surface area for segments in the model:

Arrangements of segments as they are stacked in the vertical

Direction with side length (L), width (W), and depth for segment (Dep).

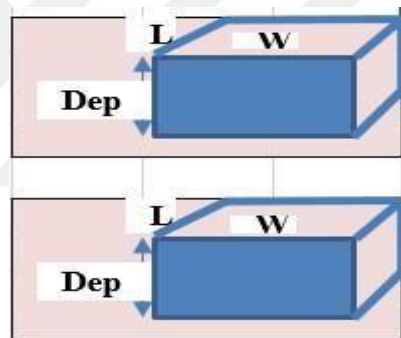


Table A4 Correlation between SOD and variables in segment 8

No.	Variable	Seg. 8	Type of correlation
1	Dissolved organic C	92.0%	positive
2	Chl-a	-80.0%	negative
3	Ammonium	-93.0%	negative
4	TP	98.0%	positive

5	TK	-87.0%	negative
6	DO	-69.0%	negative
7	CBOD	-95.0%	negative
8	Temperature	95.0%	Positive
9	Nitrate	92.0%	Positive

TABLE A5 Values of constants used for the model:

<u>Value</u>	<u>Description</u>
0.05	Maximum temperature swing during DT [Celsius]
0.5	Maximum fraction NH ₃ added by diagenesis flux during DT
0.05	Maximum growth of phytoplankton during DT [fraction]
40.16	Latitude- degrees
32.42	Longitude- degrees
3	Sediment (ground) temperature- $\hat{A}^{\circ}\text{C}$
0.01	Nitrification Rate Constant @20 degree C (1/day)
1.05	Nitrification Temperature Coefficient
2	Half Saturation Constant for Nitrification Oxygen Limit (mg O ₂ /L)
7	Minimum Temperature for Nitrification Reaction (degree C)
0.1	Denitrification Rate Constant @20 degree C (1/day)
1.05	Denitrification Temperature Coefficient
2	Half Saturation Constant for Denitrification Oxygen Limit (mg O ₂ /L)

- Dissolved Organic Nitrogen Mineralization Rate Constant @20 C
 - 1 (1/day)
 - 1.01 Dissolved Organic Nitrogen Mineralization Temperature Coefficient
 - 0.02 CBOD Decay Rate Constant @20 C (1/day)
 - 1.03 CBOD Decay Rate Temperature Correction Coefficient
 - 0 CBOD Half Saturation Oxygen Limit (mg O₂/L)
 - 0.65 Fraction of Detritus Dissolution to CBOD
 - 0 Fraction of CBOD Carbon Source for Denitrification
 - 7 The Reaeration Rate when temp. at 20 °C (1/day)
 - Options for reaeration calculations: [zero @ Covar], [1@Connor], [2@Owens], [3@Churchill] and [4@Tsivoglou]
 - 33 Reaeration Rate [day⁻¹] the Maximum rate
 - 2 The type of water body
 - 400 Bottom sediment light thresh hold(watts/m²)
 - Max. allowable growth rate for Phytoplankton at a constant temp of 20 °C per day
 - 1 Temperature growth rate
 - 100 The ratio of Carbon to Chlorophyll (mg C/mg Chl)
 - 20 Absolute optimum temp.
 - 0.29 Respiration constant for growth per day at the constant temp.
 - 1.06 Respiration Coefficient for ambient temp.
 - 0 Death Rate Constant per day Phytoplankton
 - 0 Grazing Rate Constant per day for Zooplankton

- 0 Grazability (0 to 1)
- 0 No Nitrogen fixation
- 1 with Nitrogen fixation
- 150 PAR Phytoplankton Light Saturation
- 0 Mineralization Rate (mg Phyt C/L)
- 0.02 N Uptake (mg N/L) at Phytoplankton
- 0.02 P Uptake (mg P/L) at Phytoplankton
- 0.2 Recycled to Organic N
- 0.2 Recycled to Organic P
- 1 Detritus N result from death of phyto.
- 1 Detritus P result from death of phyto.
- 4 Detritus to Carbon Ratio (mg D/mg C)
- 0.22 Nitrogen to Carbon Ratio (mg N/mg C)
- 0.15 Phosphorus to Carbon Ratio (mg P/mg C)
- 1 Diel light Option
- 1 Type of model is active sediment
- 1 no steady-state calculation sets initial conditions
- 0.001 Acceptable error
- 1000 Iteration number above this value
- 0.2 Quantity of solids at Layer 1 kg/L
- 0.1 Layer thickness
- 0.3 Quantity of solids at Layer 2 kg/L
- 0.002 The rate of diffusion between layer 1 and layer 2 (m²/day)

1.01 Correction coefficient of D_p

1.1 Coefficient of D_p

0.27 Rate at particle mixing

4 Oxygen saturation



APPENDIX B

OUTPUT RESULTS OF WASP8

Samples

R^2 measures the strength of the relationship between our model and the dependent variable. Presented in the graphs below for all the state variables:

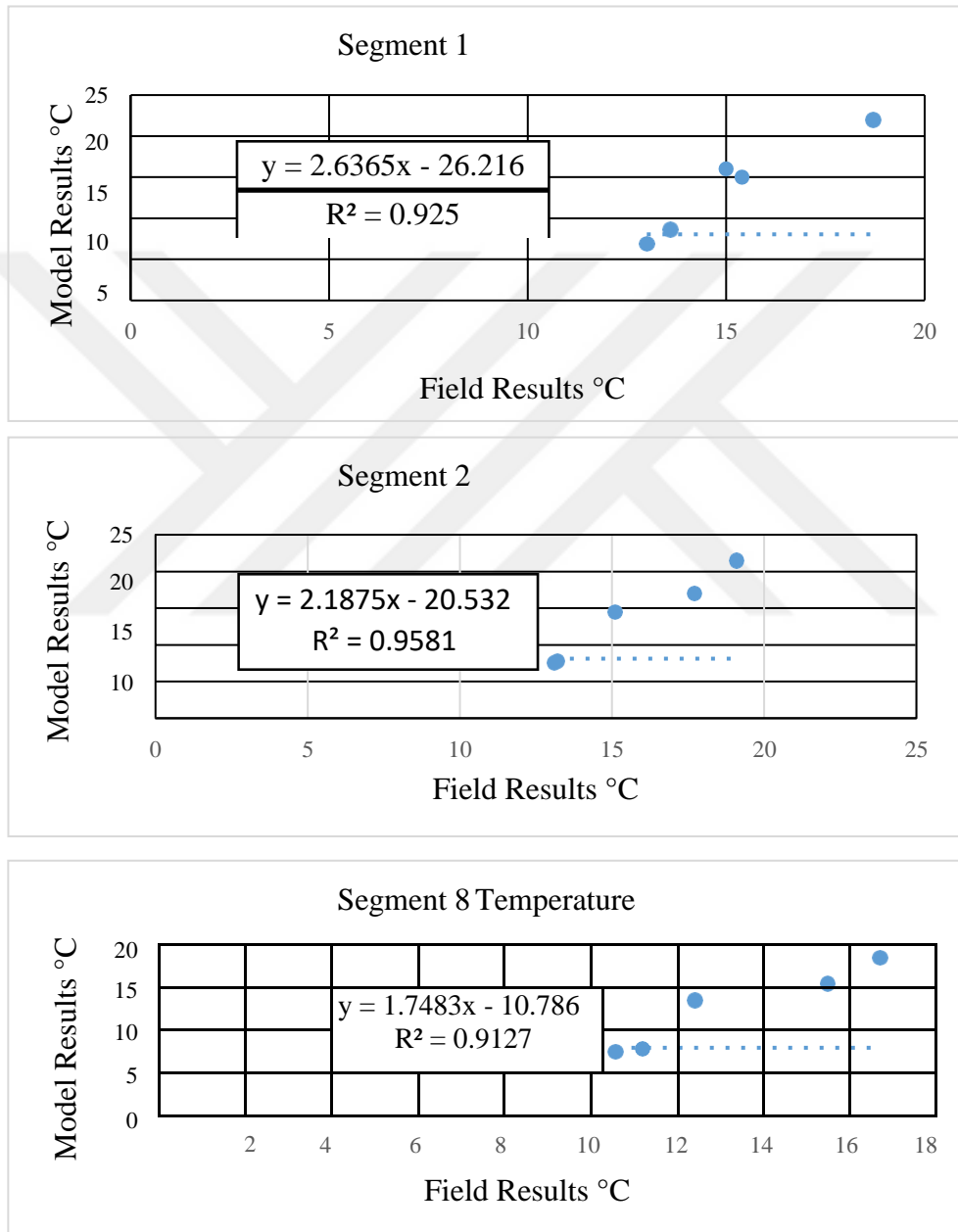


Figure B1 correlation between model results and field measurements for temperature at seg.1, 2 and 8

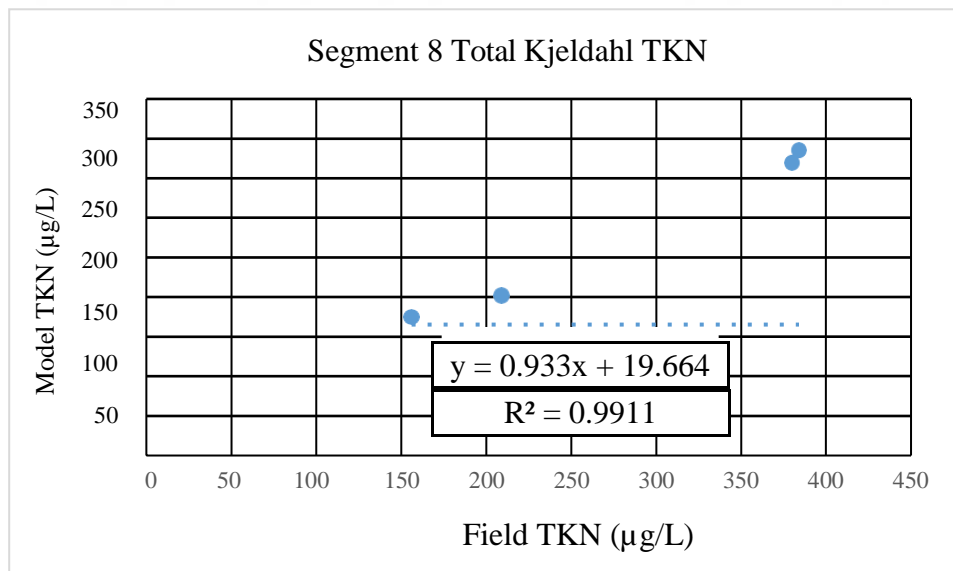
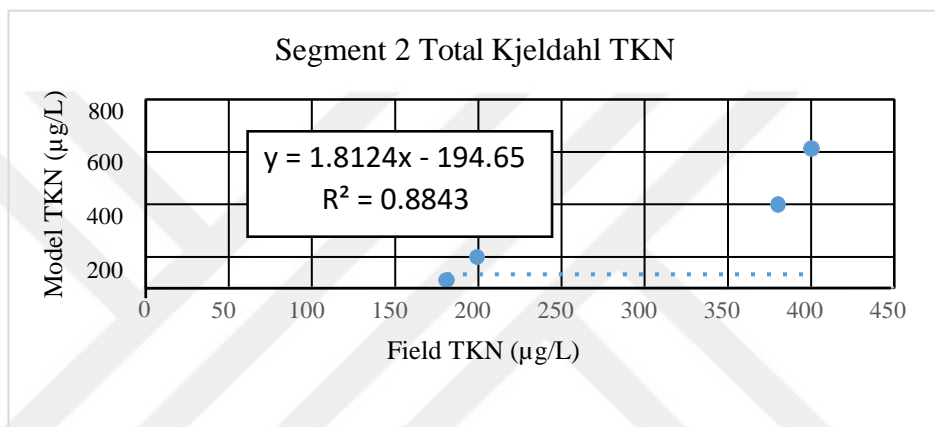
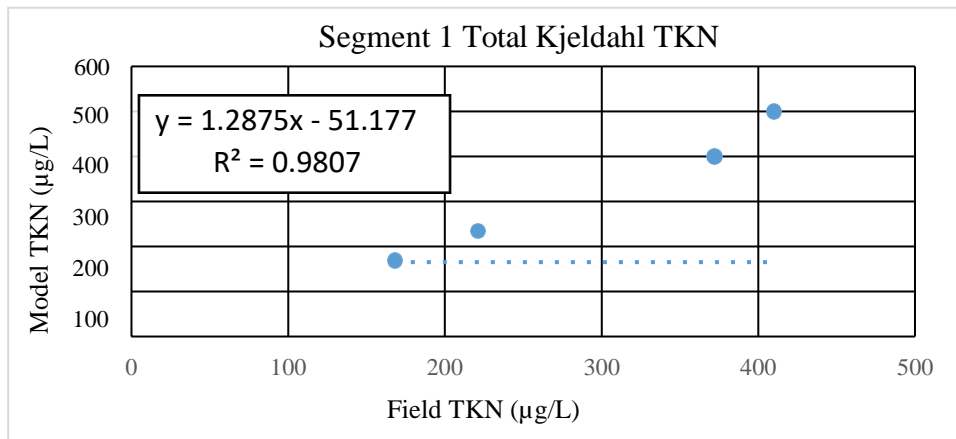


Figure B2 correlation between model results and field measurements for total kjeldahl at segment 1, segment 2 and segment 8

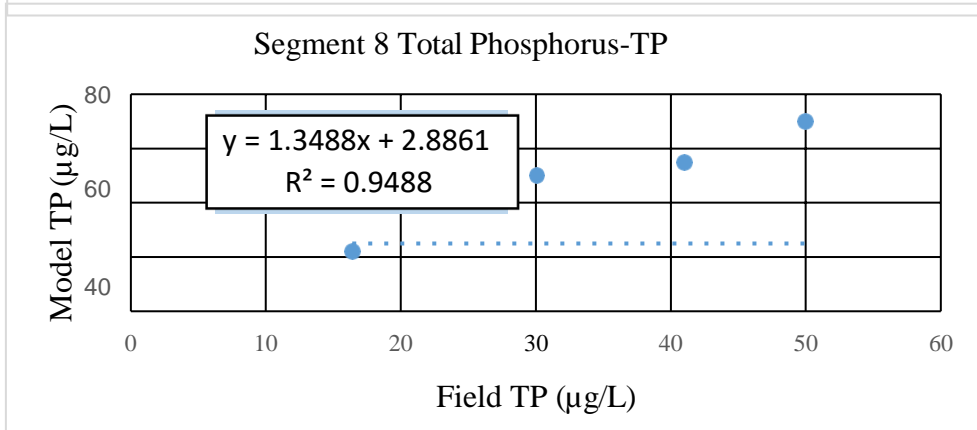
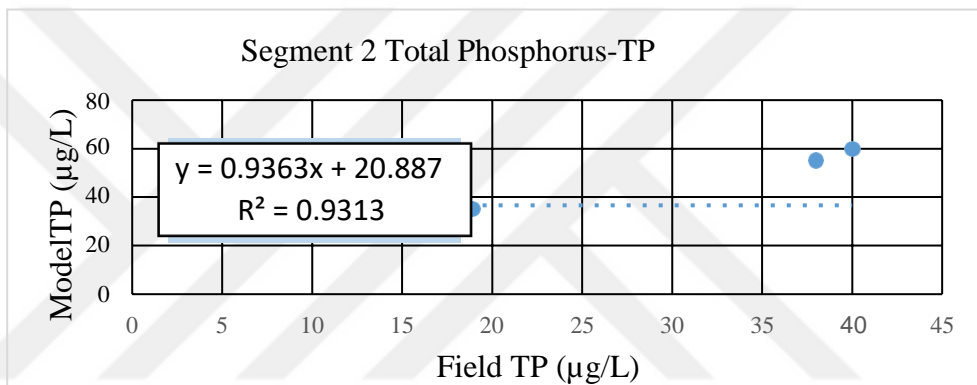
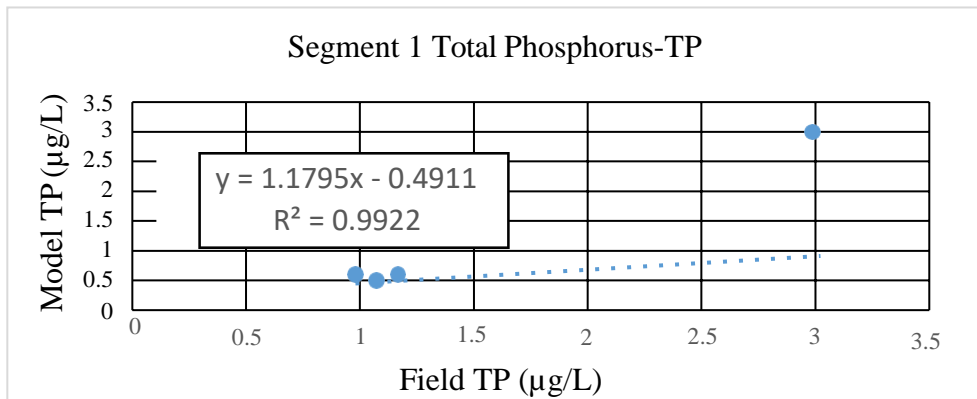


Figure B3 correlation between model results and field measurements for total phosphorus at segment 1, segment 2 and segment 8

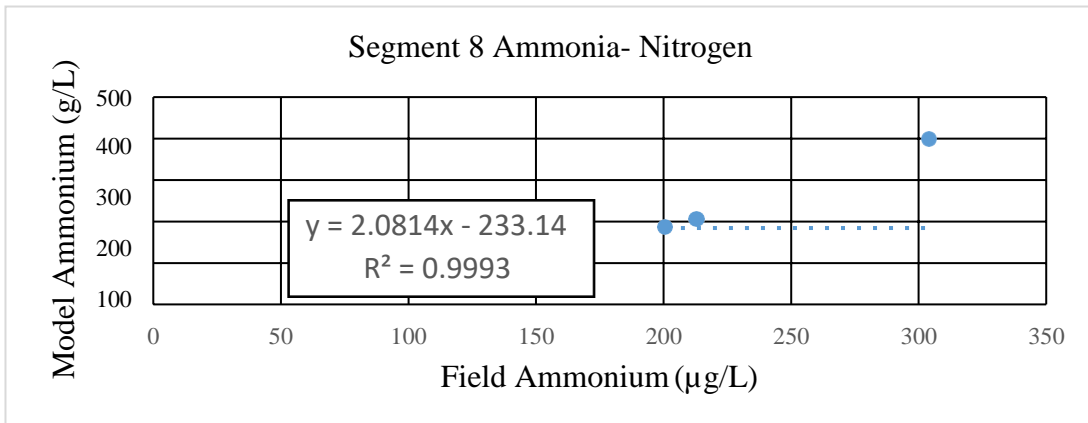
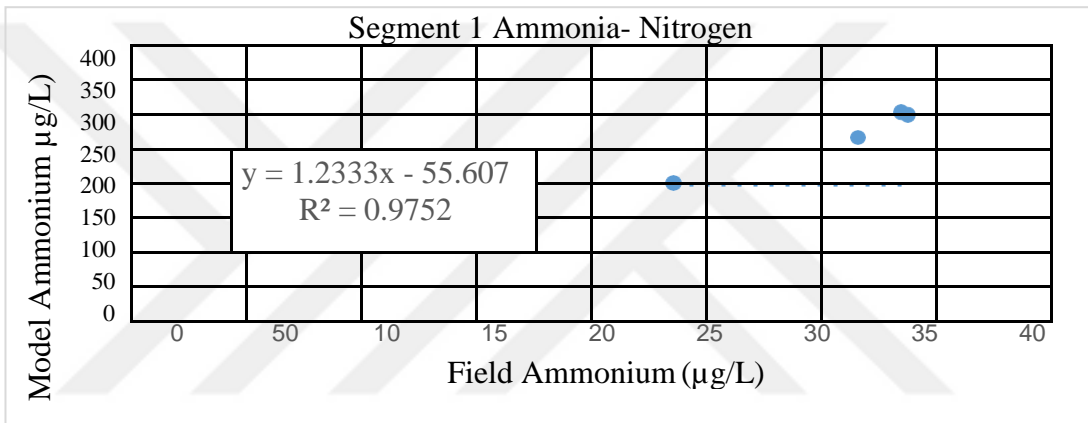
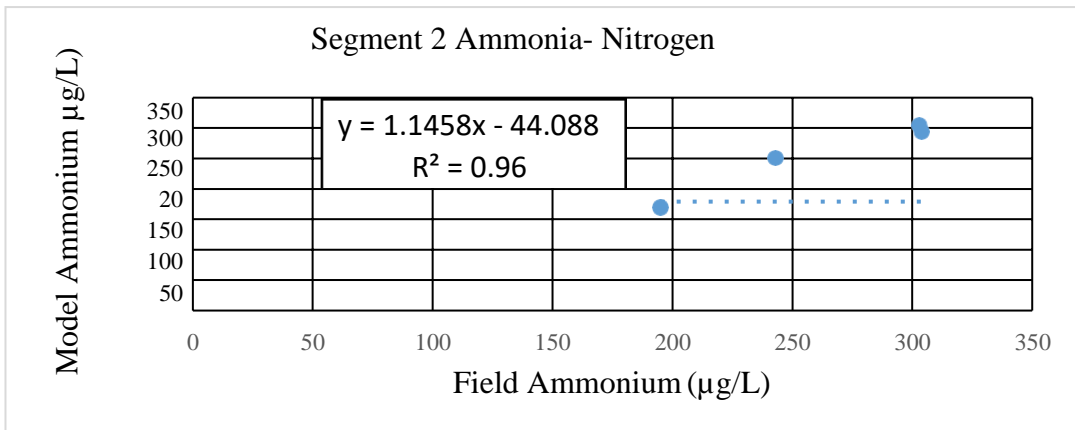


Figure B4 correlation between model results and field measurements for ammonium at segment 1, segment 2 and segment 8

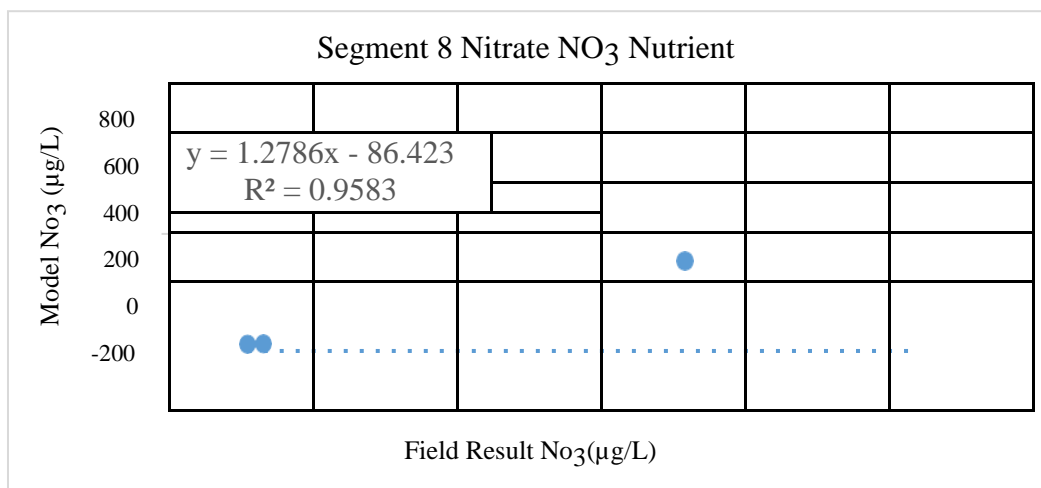
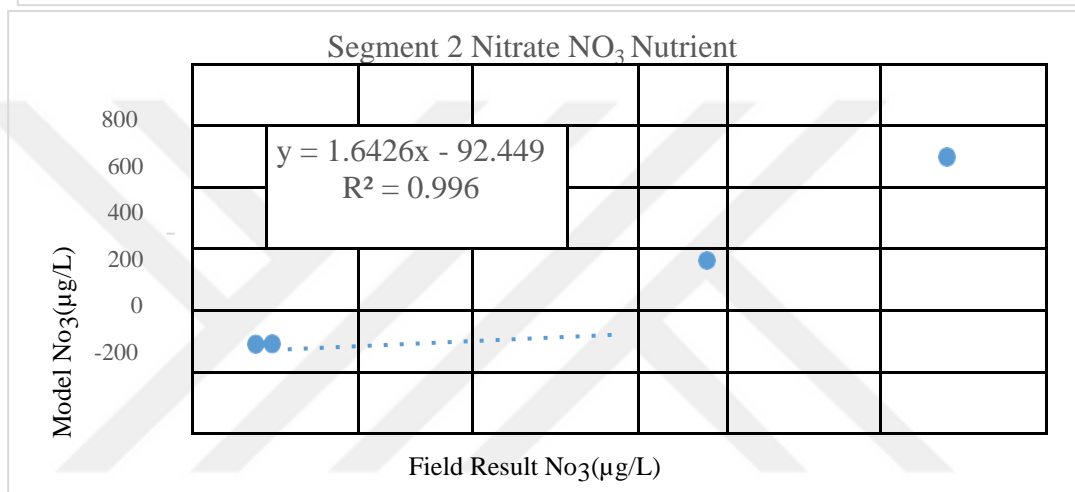
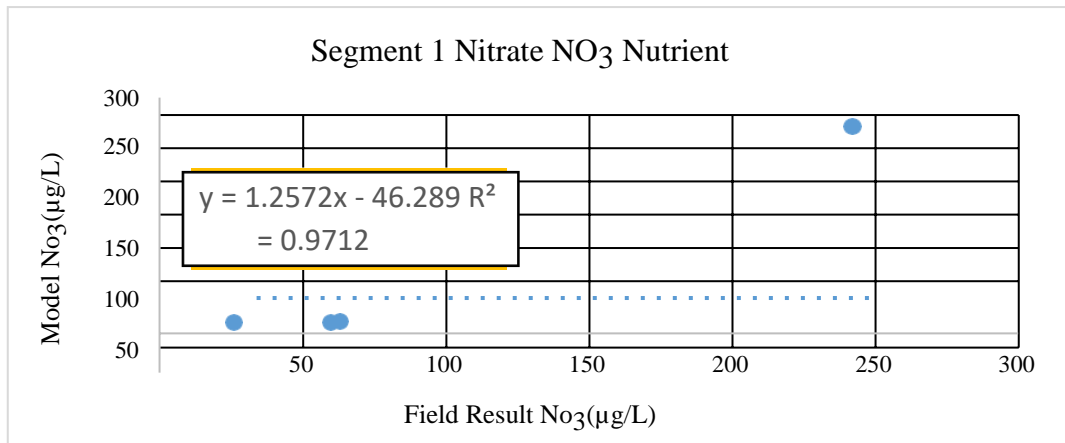


Figure B5 correlation between model results and field measurements for nitrate at segment 1, segment 2 and segment 8

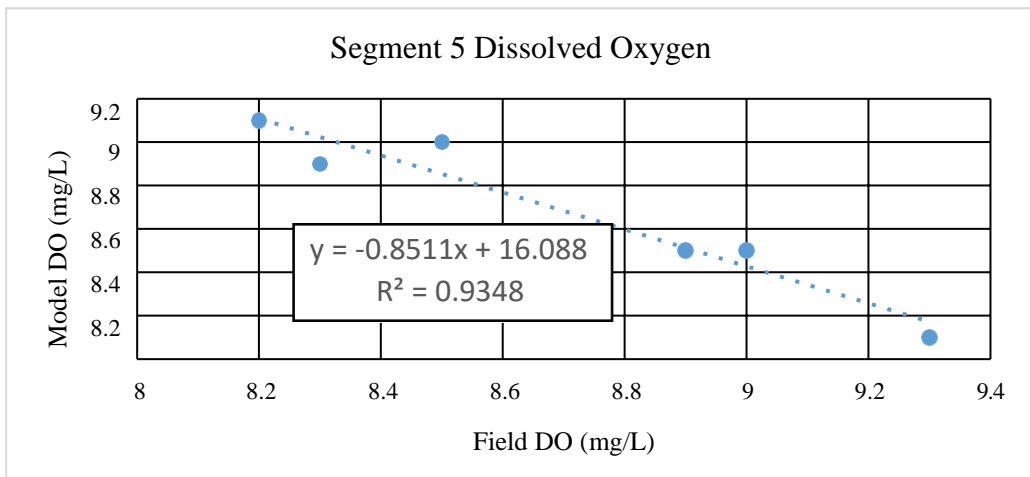
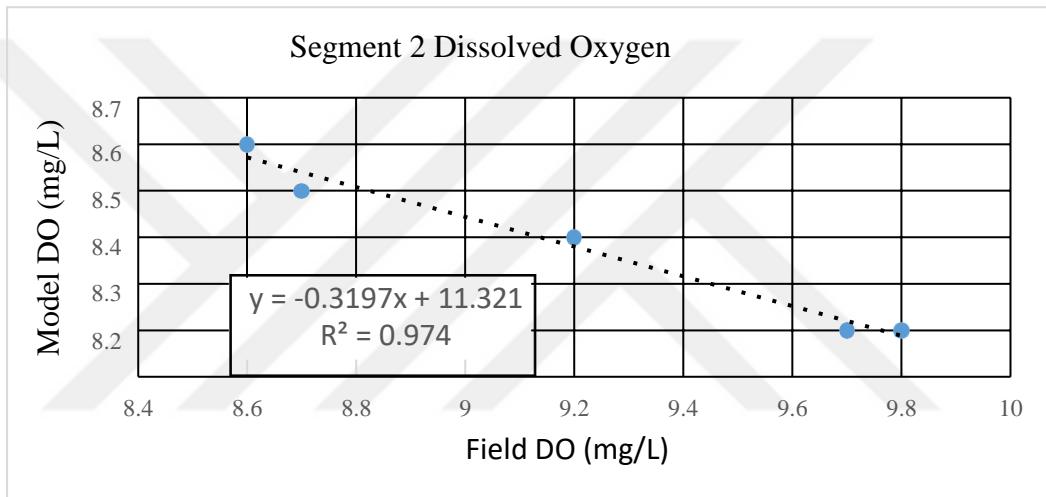
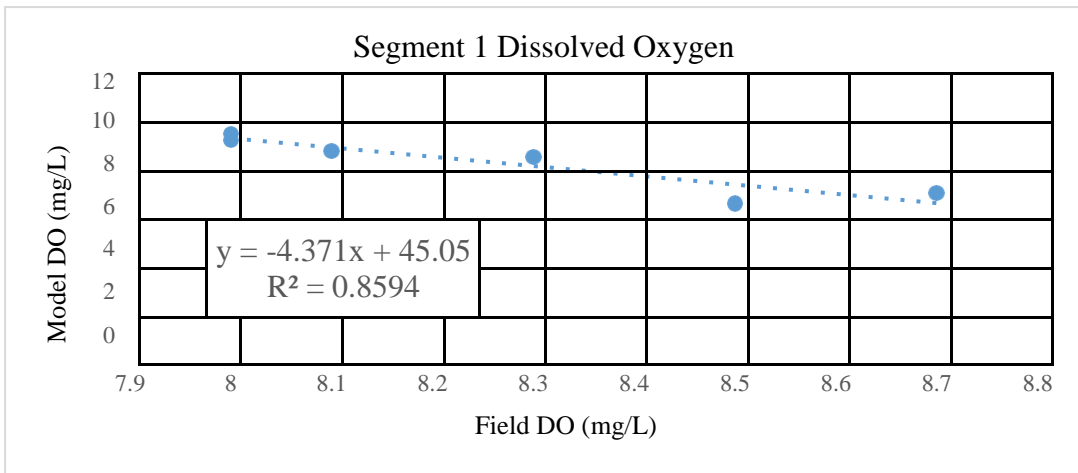


Figure B6 correlation between model results and field measurements for dissolved oxygen at segment 1, segment 2 and segment 8

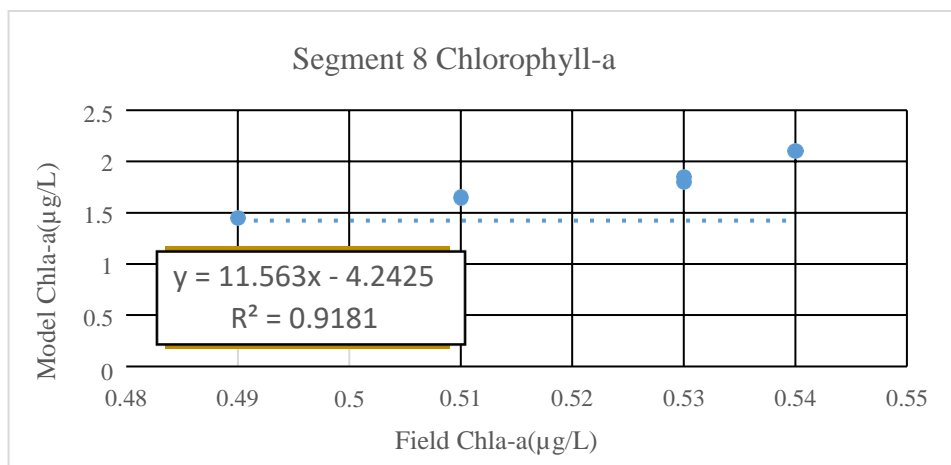
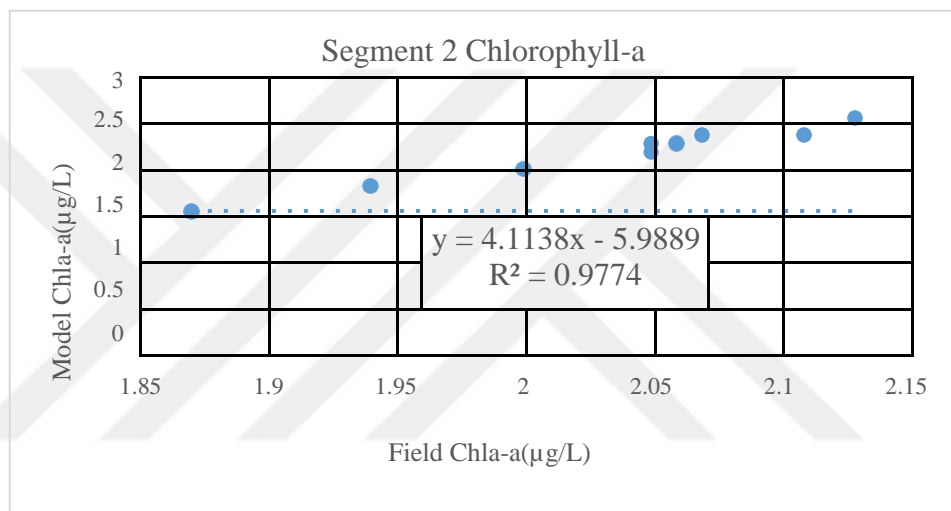
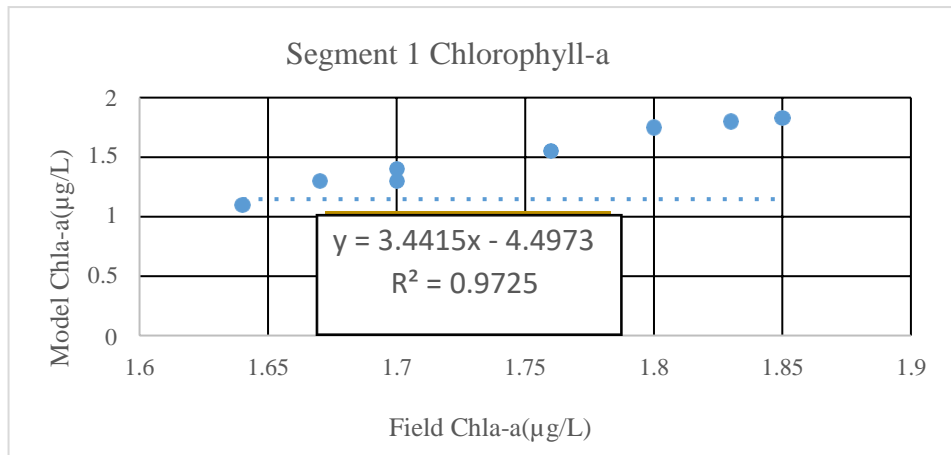


Figure B7 correlation between model results and field measurements for chlorophyll-a at segment 1, segment 2 and segment 8

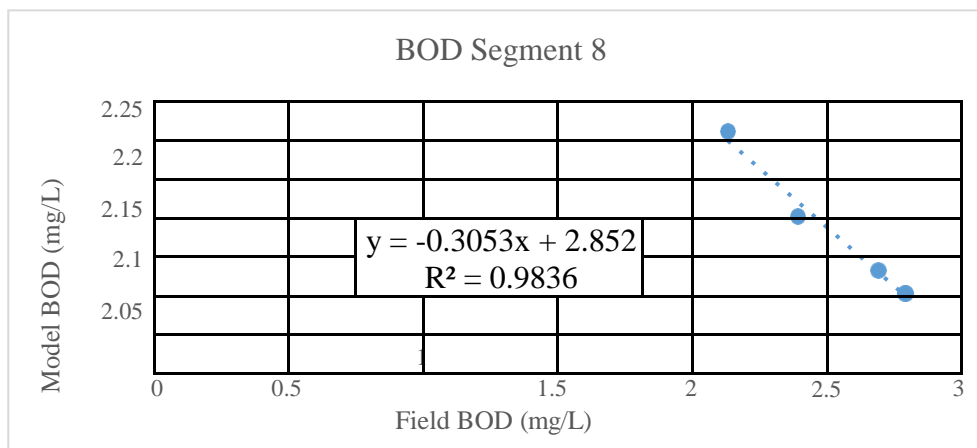
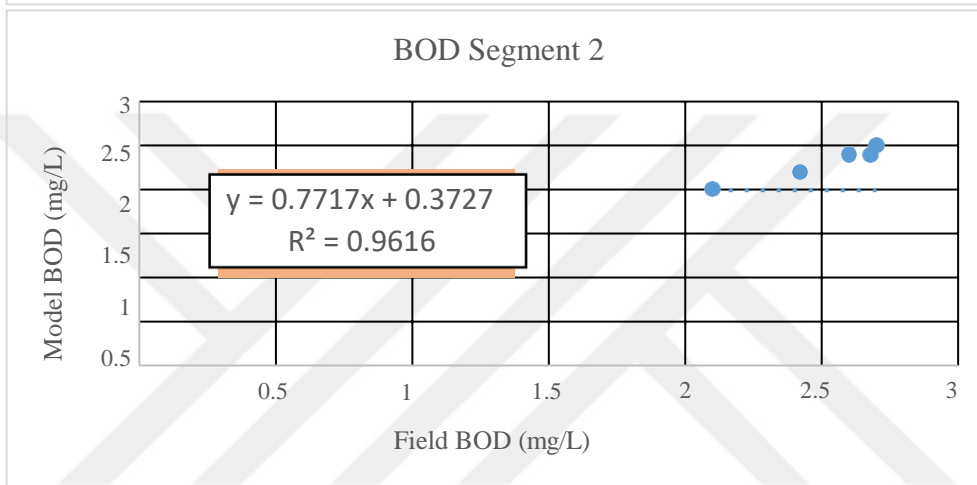
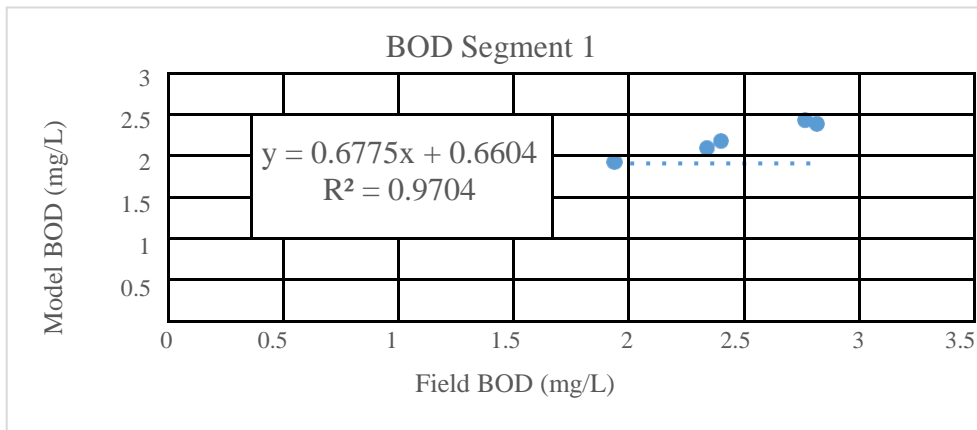


Figure B8 correlation between model results and field measurements for BOD at segment 1, segment 2 and segment 8

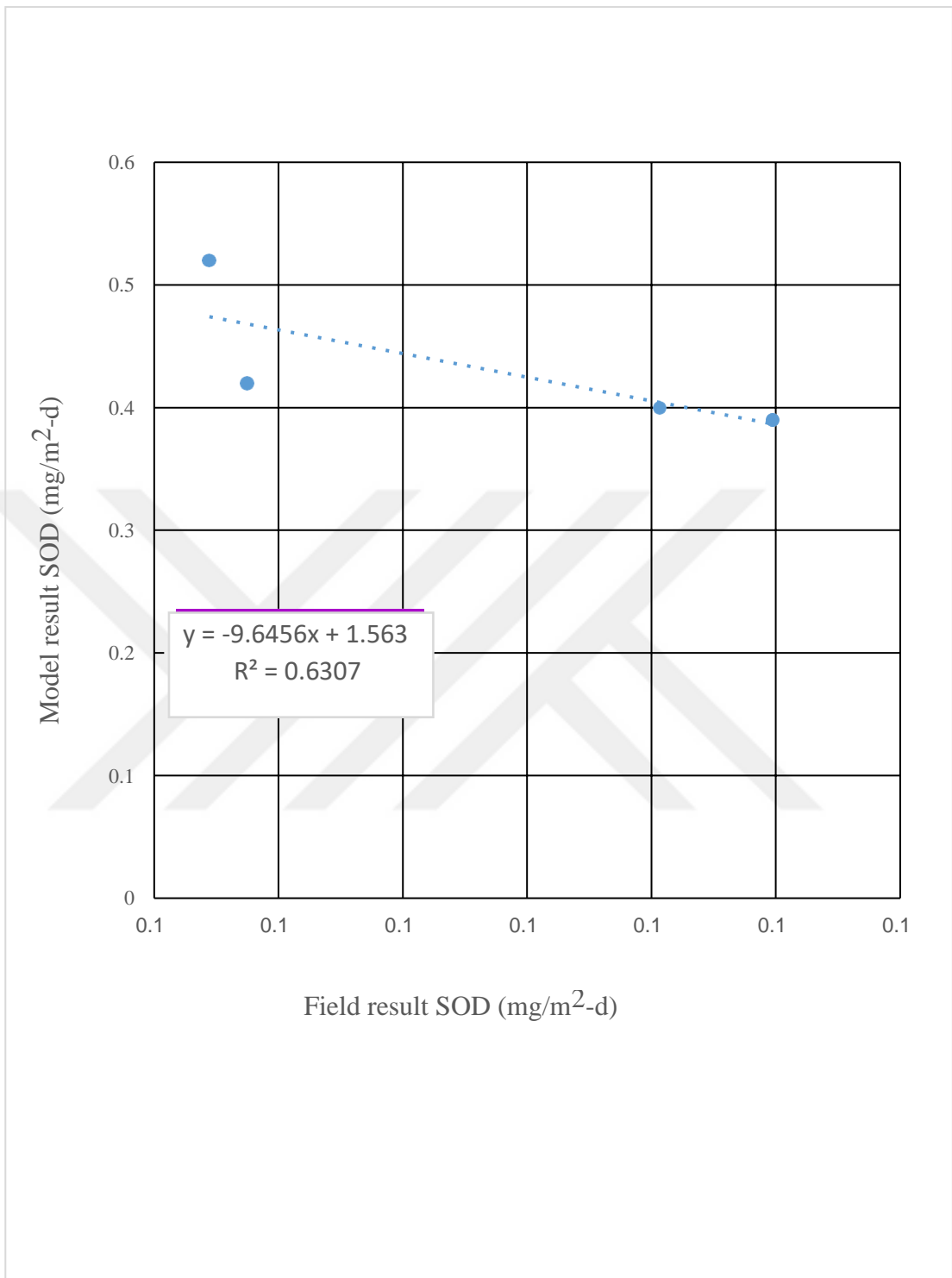


Figure B9 correlation between model results and field measurements for SOD at segment 1

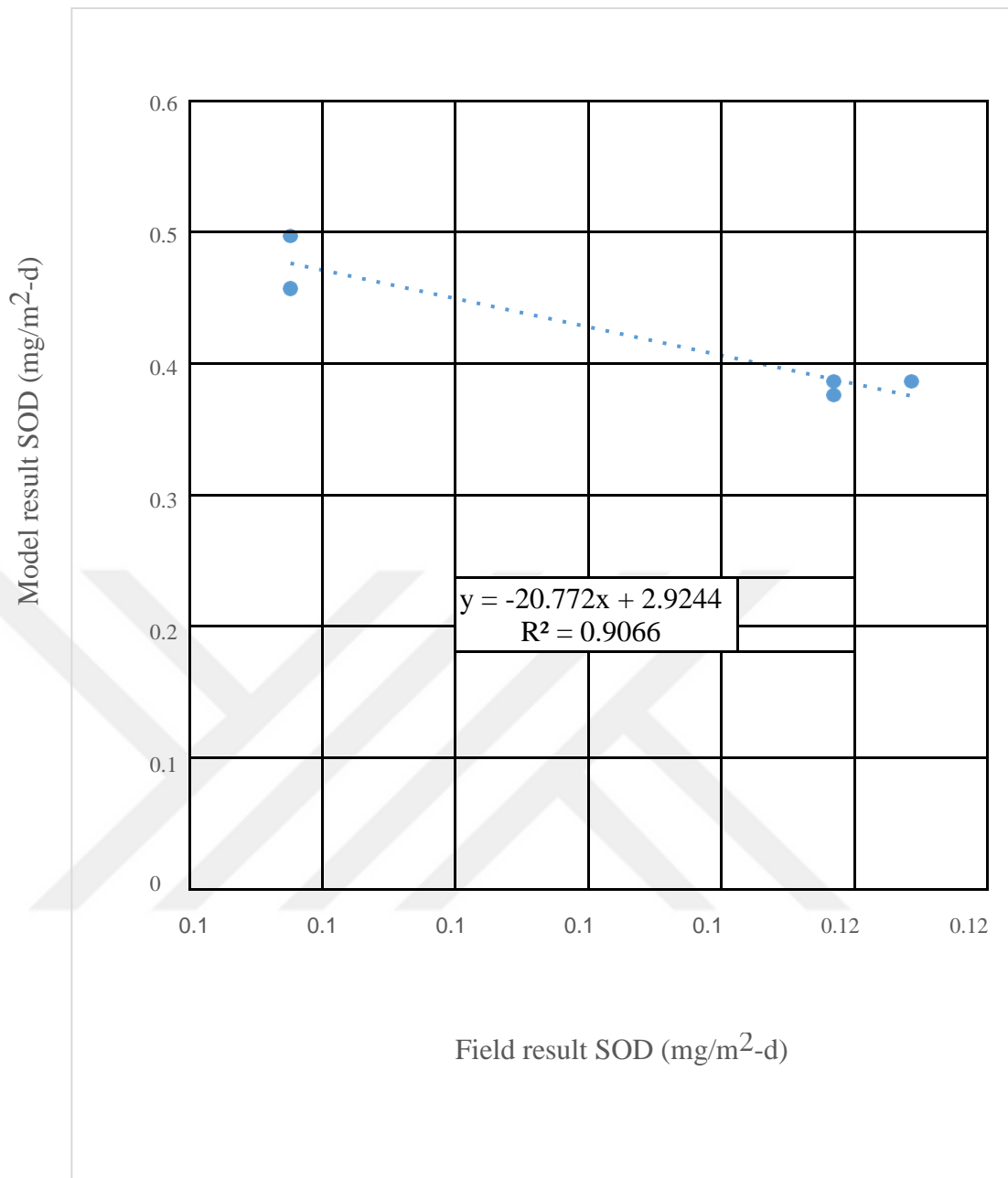


Figure B10 correlation between model results and field measurements for SOD at segment 2

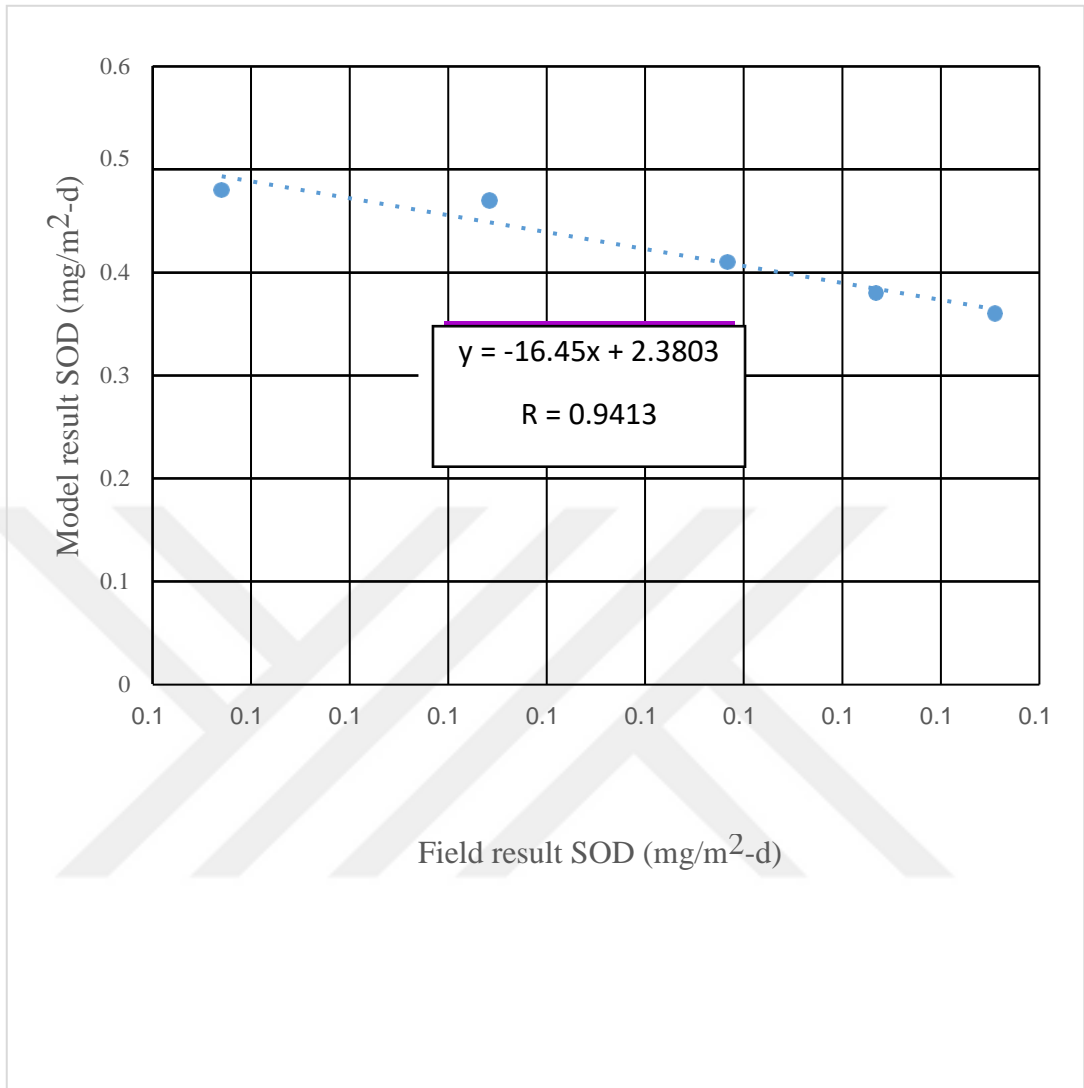


Figure B11 correlation between model results and field measurements for SOD at segment