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Simulation modeling of nutrients, dissolved oxygen and total dissolved solids in Peer-Bazar River and Anzali wetland eutrophication prediction

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ABSTRACT

The Peer-Bazar river delivers pollutants in the water bodies of Anzali International Wetland especially during flood events. Here, the two-dimensional (2D) finite volume hydrodynamic models for the prediction of nutrients are developed. The model is based on the mass balance equation including advection and diffusion transport and chemical and biological transformation considering the impact of inflowing river and climate change. The model is formulated to simulate nutrients such as Amonia-Nitrogen (NH_3–N), Nitrate (NO_3–N) or overall Total Nitrogen (TN), Phosphorus (PO_4^{3-}) or TP, Dissolved Oxygen (DO) and Total Dissolved Solids (TDS) and prediction of spatial and temporal distributions of concentration of each parameter in the Peer-bazar estuaries leading to the Anzali International Wetland. Ten points of the Peer-bazar River were studied during an 18-month period from June 2014 to December 2015. The simulation and numerical analysis of water quality parameters were conducted in a 2-dimensional approach using the geometric and topographic data and imposing boundary conditions. This research used the software developed by the author, FLOW-3D mathematical model, and HEC-RAS for simulation and qualitative evaluation of the river. Results revealed that the mean concentration of phosphorous, nitrogen and TDS exceeded the permissible limits reported by the European Directive 80/778/EEC and OECD and USEPA standards. Therefore, water of the region is subject to the advanced eutrophic conditions. Simulation predictions showed that the variation in TDS and nutrients contents will increase in the next coming years and the region will reach to the stable conditions. Using regression, a relationship between EC and TDS was obtained in the next step. Comparing the results obtained by the simulator and the values measured in laboratory indicated the suitable performance of reference values.

Keywords: Simulation and numerical analysis; Hydraulic flow; The finite-volume method (FVM); Peer-Bazar River

1. Introduction

Rivers are among the most principal water resources, important and vulnerable inland ecosystems [1]. Today, the quality of such water resources has been threatened, due to either irregular consumption of water or pollution with industrial and municipal wastewaters [2]. With respect to the importance and vital role of rivers in supplying required amount of water for human and the other objectives, it is essential to study concentration of pollutants to control and protect water resources. Simulation would be an effective approach in studying the effect of each pollutant source and predicting the impact of adding loading resources. HSPF, AGNPS, CORMIX, SLAMM, ANSYS FLUENT, QUAL2KW and families of WASP and MIKE are among the most common simulators in water quality issues. All the simulators deal with solving the mass balance equation and QUAL2E and WASP have performed well on simulating water quality of rivers [3–6].

In the present study, a Flow-3D (10.1. Ink) mathematical model (software) was applied. Comparing with

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the other similar engineering software, this software is authenticated and popular [7]. One of the unique features of the simulator is providing outstanding graphic results, as it is capable of exhibiting animation and dynamics behavior of fluids appropriately in 2D and 3D. Mirbagheri et al. [8–16] modeled water quality parameters in rivers, lakes, reservoirs and wetlands. Most lake and wetlands water quality models make simplifying hydrodynamic assumptions, erg. The river, lake and wetlands are well mixed.

The innovative points of this research that distinguish it from the other performed studies are presented as follows:

1. Up to now, the two-dimensional numerical and mathematical models of hydraulic streams discharging into the rivers for finding the concentrations of contaminants have not been studied. Therefore, this is the first study that used this model for the abovementioned purpose (Until now, for determination of contaminants in surface and river waters, the conceptual, non-dynamic and one-dimensional models have been used).
2. In addition, this model can exhibit animation and dynamics behavior of fluids to monitor the transport and diffusion of contaminants in water resources and find their temporal and spatial distributions at different climate conditions with high speed and accuracy. However, based on previous research, the capabilities have not been observed in previous studied models.
3. Moreover, by using the developed software prepared by the authors of this research, this is the first time that the forecasting of the quality of river water discharging into Anzali international wetland (Peer-bazar River in north of Iran) at both present and future was carried out which showed the advanced eutrophic conditions of water quality. The obtained results of forecasting by using this software revealed that the mean annual concentrations of ammonium, nitrate, nitrite, phosphate and dissolved ions in river water will be increased by 1.2, 3.2, 32, 5 and 7% in 2022, respectively. These values will be increased to 3.4, 9, 87, 14 and 16.6% in 2032, respectively, which is an innovation in water pond quality management.

Literature shows that Peer-bazar River is one of the most important rivers feeding the Anzali international wetland [17]. In 1997, the obtained data showed that the annual means of sediments, nitrogen, phosphorus, and phosphate discharged into the river were 86000, 931, 184, and 21.3 tons, respectively [18]. Studies showed that 1.34 million square meters of untreated wastewater discharged into the Anzali wetland through Peer-bazar River [19].

This research aims at simulating and carrying out numerical analysis of concentration distribution of nutrients, DO and TDS parameters and examining the dynamic behavior of river water flow and 2D equations of hydraulic flow of direction and water flow rate on changes of concentration of each parameter in the estuaries of the Peer-bazar River. Other research objectives were included simulation, experimental measurement, examination and identification of pollutant resources, prediction of the present and future conditions of qualitative parameters of river using the software developed by the authors, application of FLOW-3D mathematical model to reduce time of study, and evaluation of each parameter and all heavy costs of sampling.

2. Materials and methods

2.1. Study location

The Peer-bazar River is located in the southeast of the Anzali international wetland in Gilan Province, Iran (Fig. 1). The river transfers industrial, hospital, agricultural, and fishery (aquaculture) wastewaters into the wetland. The wastewater includes all types of pollutants such as heavy metals, nutrients, etc. [20].

2.2. Field data

To conduct the study, the sampling process was carried out at ten points of the Peer-bazer River estuaries between Ghalam Goodeh and Sooser downstream (due to the flow of pollutant resources in this area) in a distance about 5 kilometers for 1D and 2D simulations of an unsteady flow (Fig. 2). Sampling was performed during 18 mo from June 2014 to December 2015. To execute simulation, the data were divided into two groups. First group (data of the 12 mo of

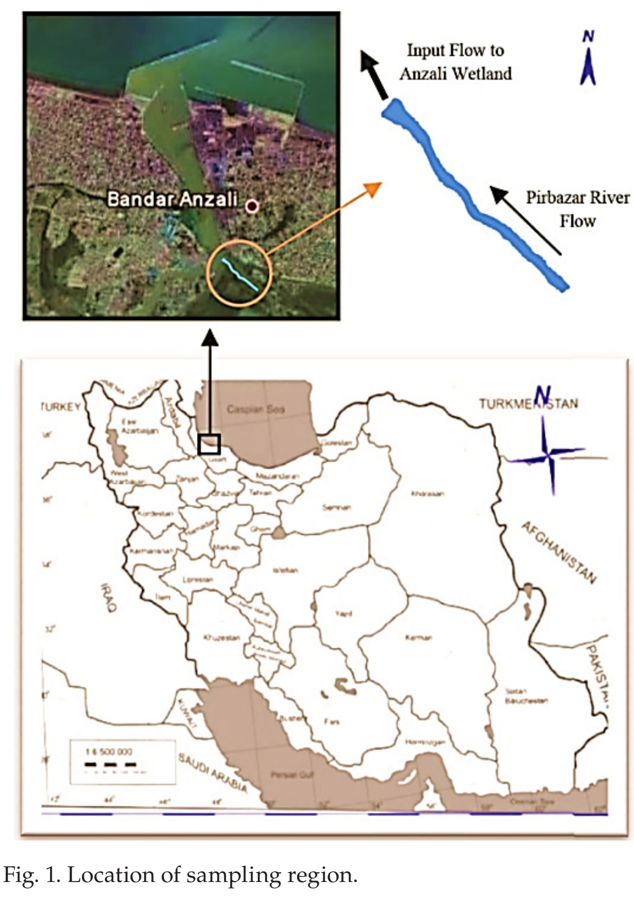


Fig. 1. Location of sampling region.

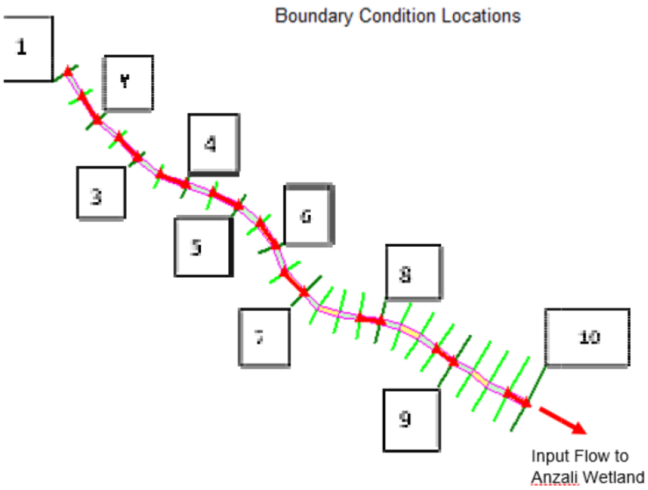


Fig. 2. Distribution of the sampling points in the study region.

the first year) was used for calibration and the second group (data of the 6 mo of the second year) was applied for test and verification.

The samples were taken at mid-season using several one-liter polyethylene containers from different depths of water (1–3 m). A small boat was used for minimizing turbulence during the sampling. In addition to the main parameters related to nutrients and TDS, the other parameters including bed depth, water temperature, air temperature, pH, dissolved oxygen, and electrical conductivity (EC) were recorded using a multi-parameter machine model 8603 by a DR 5000 TM UV-VIS Spectrophotometer model Hatch.

Bottles containing the collected samples were consolidated in the sampling site as per the standard method [21] for verification of the model in terms of the type of measureable parameter. Then, they were then transferred to the laboratory of Environment General Office of Gilan Province. It should be mentioned that the chemical analysis of water samples (three iterations for each parameter) was performed as per the standard method. As fluctuation is seen less in the one-dimensional results (the one-dimensional information is the same direct sampling from the natural Peer-bazar River), the results were used for the relationship between the points and removing fluctuations and non-convergence. The parameters of 2D flow and the variables of the one-dimensional flow were linked and the one-dimensional simulation results were extracted from HEC-RAS (4.1.0 Ink). (The related analysis results in *text* format were used as the input data for the two-dimensional model).

In order to evaluate the effect of climate conditions on water flood and quality, several meteorology data related to climatic parameters like precipitation in catchment, air temperature and acloud were applied in model. Based on the low distance between Peer-bazar river and synoptic station of Anzali port, the obtained data of 2000–2010 were applied. Mean annual precipitation (MNP) in this station is 1857 mm which the minimum and maximum MNP are 45.6 mm (in July) and 335.1 mm (in October), respectively. Mean air temperature (MAT) is 16.2ºC which the minimum and maximum MAT are 7.3ºC (in February) and 29.9ºC (in July), respectively. Since during 10 mo of the year the weather was cloudy, 0.9 was used as an acloud coefficient in model (0.1 is for sunny weather condition). Among the other climatic conditions, atmospheric pressure, steam pressure, speed of wind and humidity were overlooked, due to either their small effect or lack of information.

2.3. Governing equations and numerical solution method

The 2D flow governing equations, which were used to predict the concentration of the qualitative parameters of shallow water, include convection-diffusion equation [Eq. (1)] and continuity equation [Eq. (2)] are as follows [22].

$$\frac{\partial c}{\partial t} = -\left(u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x} + \left(D_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right) \pm S_c \quad (1)$$

$$\frac{\partial \zeta}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (uh)}{\partial y} = 0 \quad (2)$$

where c is the concentration of qualitative components (g/L), x,y : Cartesian directions (m), u: velocity factor along x axis (m/d), v: velocity component along y axis (m/d), D_x, D_y: impact factors in longitudinal and lateral axes (m/d), t : time (d), S_c: sources/sinks (g/m^3.d), ζ: water level, h: mean depth of water (m).

Since in Eq. (1), S_c has significant influence on the variety of nutritional elements in simulation process, the considered parameters of nutritional elements for S_c are reported below (The methodology proposed in this paper can be a useful tool for finding sources and sinks of FDOMs [23] in a riverine system influenced by natural organic matter impairment).

The different nutritional parameters were the rate constants for physical and chemical reactions between algae, nitrogen, phosphorous, dissolved oxygen and carbonaceous biological oxygen demand (CBOD). These rate constants control S_c in equation and are also dependent on temperature [24] (In Eqs. (3)–(12), temperature dependency of each parameter related to sources/sink is marked by *. Furthermore, the name and values of different nutritional parameters and their relationship with each other are reported in Table 1).

The parameter θ is qater experimental temperature correction coefficient. This coefficient is 1.024 and 1.047 for physical and chemical reactions, respectively [25].

Source/Sinks of alive algae biomass (A): The water quality model can only simulate phytoplankton algae that is buoyant on the surface of water and feed from water column. The growth and respiration of algae affect the concentrations of algae, nutrient elements and dissolved oxygen in the solution. Source/Sinks of alive algae biomass can be calculated via the equation below [26]:

$$A_{Source/\sin k} = A\mu^*_{\max}GL - A\rho^* - \frac{\sigma^*_1}{h}A \quad (3)$$

where G is the growth limitation of algae which is obtained by nutrients formulation Leibery minimum:

$$GL = FL_{\min}(FP, FN) \quad (4)$$

Table 1
The features and relationship between different parameters of nutritional parameters in water quality model

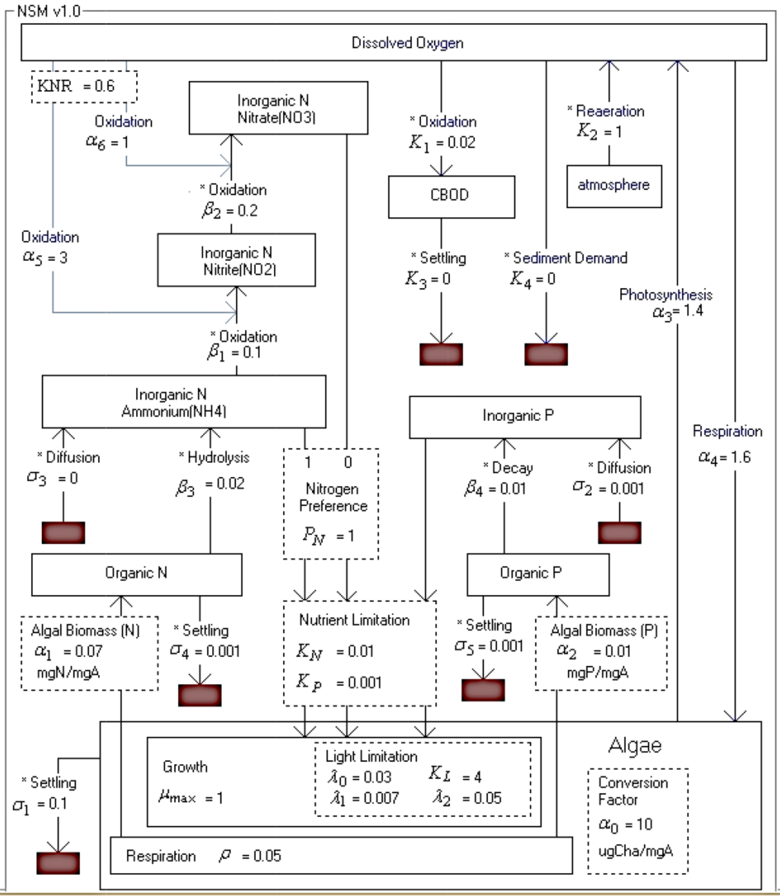
Water Quality Data

Nutrient Modeling Parameters

Restore Default Values... | View Both Table and Schematic | View Table only | View Schematic only

Algal local specific growth rate formulation: Multiplicative

Variable		Value	θ
Algae			
α_0 Biomass (Chl-a ratio)	ugCha/mgA	10	
α_1 Biomass (Nitrogen Fraction)	mgN/mgA	0.07	
α_2 Biomass (Phosphorus Fraction)	mgP/mgA	0.01	
μ_{max} Maximum Growth Rate	day -1	1	1.047
ρ Respiration Rate	day -1	0.05	1.047
P_N Nitrogen Preference		1	
K_L Growth Limitation (light)	W m-2	4	
K_N Growth Limitation (N)	mgN/L	0.01	
K_P Growth Limitation (P)	mgP/L	0.001	
λ_0 Light Extinction (non-algal)	m -1	0.03	
λ_1 Light Extinction (linear algal)	m-1(ugCh/L)-1	0.007	
λ_2 Light Extinction (non-linear algal)	m-1(ugCh/L)-2/3	0.05	
σ_1 Settling Rate	m day-1	0.1	1.024
Dissolved Oxygen			
α_3 Production per unit algal growth	mgO/mgA	1.4	
α_4 Uptake per unit algal respired	mgO/mgA	1.6	
α_5 Uptake per unit NH4 oxidized	mgO/mgN	3	
α_6 Uptake per unit NO2 oxidized	mgO/mgN	1	
K_2 Atmospheric Reaeration	day -1	1	1.024
K_4 Sediment Demand	day -1	0	1.06
CBOD			
K_1 Decay Rate	day -1	0.02	1.047
K_3 Settling Rate	day -1	0	1.024
Nitrogen			
β_3 OrgN->NH4	day -1	0.02	1.047
β_1 NH4->NO2	day -1	0.1	1.083
β_2 NO2->NO3	day -1	0.2	1.047
σ_4 Org-N Settling Rate	day -1	0.001	1.024
σ_3 NH4 Benthos Source Rate	mgN m-2 day -1	0	1.074
KNR Nitrification Inhibition Factor	mg/L	0.6	
Phosphorus			
β_4 OrgP->InorgP	day -1	0.01	1.047
σ_5 Org-P Settling Rate	day -1	0.001	1.024
σ_2 Benthos Source Rate	mgP m-2 day -1	0.001	1.074



where, FN is the nutrient limitation for nitrogen $\left(FN = \frac{NH_4 + NO_3}{NH_4 + NO_3 + KN}\right)$, FP is nutrient limitation for phosphorus $\left(FP = \frac{PO_4}{PO_4 + KP}\right)$ and FL is limitation for light $\left(FL = \frac{1}{\lambda h}\ln\frac{KL + 0.5}{KL + 0.5e^{-\lambda h}}\right)$ which λ is equal to $\lambda = \lambda_0 + \lambda_1\alpha_0 A + \lambda_2(\alpha_0 A)^{\frac{2}{3}}$.

Sources/sinks of dissolved organic nitrogen (OrgN): Various forms nitrogen such as $N–NH_3$, $N–NO_3$, $N–NO_2$ and organic nitrogen are present in the river water. The only internal source of organic nitrogen in the model is the algae respiration. The sinks of organic nitrogen are sedimentaion and hydrolysis for production of ammonia nitrogen. The sources/sink of organic nitrogen are as follows [27]:

$$OrgN_{Source/\sin k} = \alpha_1\rho^* A - \beta_3^* OrgN - \sigma_4^* OrgN \quad (5)$$

Sources/sinks of ammonia nitrogen (NH_4): The internal sources of ammonia nitrogen are organic nitrogen hydrolysis and dispersion from benthos. Their internal consumptions are oxidation of ammonium to nitrate and application by algae. Sources/sinks of ammonia nitrogen are calculated via the following equation:

$$NH_{4Source/\sin k} = \beta_3^* OrgNA + \frac{\sigma_3^*}{h} - \beta_1^*(1 - \exp^{-KNR-DO})NH_4 - F_1\alpha_1\mu A \quad (6)$$

where, F_1 is part of adsorbed ammonium by algae and its amount is equal $F_1 = \frac{P_N NH_4}{P_N NH_4 + (1 - P_N)NO_3}$

Sources/sinks of nitrite nitrogen (NO_2): The major source of nitrite is the oxidation of ammonium to nitrite. The only sink of nitrite is its oxidation to nitrate. Sources/sinks of nitrite nitrogen can be determined via the equation below:

$$NO_{2Source/\sin k} = \beta_1^*(1 - \exp^{-KNR.DO})NH_4 - \beta_2^*(1 - \exp^{-KNR.DO})NO_2 \quad (7)$$

Sources/sinks of nitrate nitrogen (NO_3): The only source of nitrite nitrogen consumption is the oxidation of nitrite to nitrate. Furthermore, the only sink of nitrite nitrogen is its consumption by algae. Sources/sinks of nitrate nitrogen are determined using the following equation:

$$NO_{3Source/\sin k} = \beta_2^*(1-\exp^{-KNR.DO})NO_2 - (1-F_1)\alpha_1\mu A \tag{8}$$

Sources/sinks of organic phosphorous (OrgP): The only source of nitrite nitrogen consumption is the algae respiration. The internal consumptions of organic phosphorous are phosphorous degradation for orthophosphate production and sedimentation. Equation below is used for finding Sources/sinks of organic phosphorous as follows [28]:

$$OrgP_{Source/\sin k} = \alpha_2\rho^* A - \beta_4^* OrgP - \sigma_5^* OrgP \tag{9}$$

Sources/sinks of orthophosphate (PO_4): Two important sources are reported for dissolved orthophosphate. One of them is orthophosphate degradation and another is its dispersion from benthos. The only consumption source of orthophosphate is its adsorption by algae. The following equation is applied for finding the Sources/sinks of orthophosphate:

$$PO_{4Source/\sin k} = \beta_4 OrgP + \frac{\sigma_2^*}{d} - \alpha_2\mu A \tag{10}$$

Sources/sinks of carbonaceous biological oxygen demand (CBOD): The sinks of this parameter are sedimentation and degradation with oxidation which are obtained using Eq. (11). But, the effect of carbon and silica cycles on this factor was overlooked, due to the low concentration of this material.

$$CBOD = -K_1 CBOD - K_2 CBOD \tag{11}$$

Sources/sinks of dissolved oxygen (DO): The sources of dissolved oxygen are atmospheric aeration and photosynthesis of algae. However, DO sinks are algae respiration, sediment oxygen demand, carbonaceous biological oxygen demand (CBOD) and oxidation ammonium and nitrite. Sources/sinks of dissolved oxygen are determined as follows:

$$\begin{aligned} DO_{Source/\sin k} &= K_2^*(O_{sat} - DO)A(\alpha_3\mu - \alpha_4\rho) \\ &\quad - K_1 CBOD - \frac{K_4}{h} - \alpha_5\beta_1 NH_4 - \alpha_6\beta_2 NO_2 \end{aligned} \tag{12}$$

The finite-volume and fractional step methods were used in this research for discontinuing and solving the governing equations. The governing equations for the computer model for two-dimensional hydrodynamic of flow are the same Eqs. (1) and (2). To solve the equations, the topography data of waterway bed (exceeding 14,016 pieces of data) were formulated in ASCII format in the software. A rectangular block was used for the solution network (Fig. 3).

The block consists of 10,800 cells in 60 m long, 20 m wide, and 3 m deep. Problem's boundary conditions were defined in a way that the specified velocity was used in the field's inflow boundary (X min) and continuative velocity was used in the field's outflow boundary (X max). Other flow boundaries were selected among symmetry types.

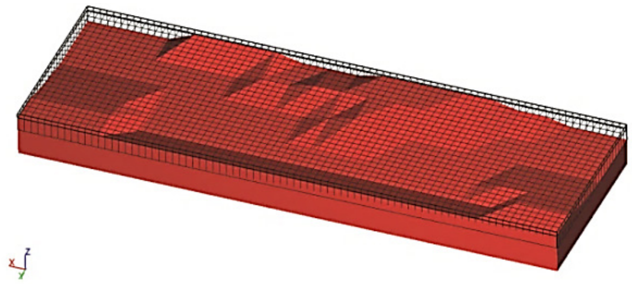


Fig. 3. Computational field, number of elements, and geometry of the study region.

In addition, Locally One Dimensional (LOD) method was used for accelerating model computations.

Since the study area was Peer-bazer River estuaries between Ghalam Goodeh and Sooser downstream, one and two-dimensional flows were simulated using HEC-RAS and Flow-3D software, respectively. In other words, all parts study region, which was explained in paragraph 2.2, were simulated using one-dimensional and two-dimensional simulators [29].

In this regard, a one-dimensional model was prepared using HEC-RAC software and the results were applied in the text format as an input information for preparation of two-dimensional model (the one-dimensional information can be considered as the measured data of river water quality parameters). The results of two-dimensional model were revised, if necessary. For example, "flow velocity" and "water level" were revised as follows:

Modification of flow velocity and water level: According to the results of two-dimensional simulation, the passed flow and mean of water level of calculated section were compared with the obtained similar parameters from one-dimensional model.

$$Q_{i_{1D}} = \sum_{j=1}^{j_{y_{\max}}} Q_{i,j_{2D}} \tag{13}$$

$$H_{i_{1D}} = \frac{1}{j_{y_{\max}}} \sum_{j=1}^{j_{y_{\max}}} H_{i,j_{2D}} \tag{14}$$

where Q_{i1D} and H_{i1D} are respectively the input flood and water level in section i in one-dimensional model. $Q_{i,j2D}$ and H_{i1D} are input flow and water level from element j in section i in two-dimensional model, respectively and J_{ymax} is the number of elements in section i in two-dimensional model. If the differences in the amount of above equations are higher than the required accuracy, the modified values of flow velocity and water level will be solved by the equation to reach the required accuracy.

2.4. Developed experimental model

Both the FLOW-3D mathematical model and the software developed by the authors were used in modeling of the research for predicting the concentration of water quality parameters. Five interpolation methods namely Kriging, Inverse distance to power, Polynomial regression, Local polynomial and S-plus were applied to find the quality of river and pond water in the next decades using the developed software. The applied approaches were compared via Cross-validation method based on root-mean-square error and the best interpolation method was selected (based on Fig. 4 which was replaced with previous flowchart). The second-order polynomial regression (with RMSE of 0.2075 and 0.1475 for total nitrogen and total phosphorous, respectively) was the best model and local polynomial model with power of 10 was the worst method, compared to the other applied approaches. Therefore, all the interpolation and extrapolation calculations in *Code Blocks* were carried out based on this method (second order polynomial regression method). The software was prepared using C^{++} programming language and it used the mean of the experimental measurement obtained in this research.

3. Results and discussion

Table 2 shows a summary of the descriptive statistics of the measured variables of water samples in 10 stations of the river with the recommended levels and the maximum permissible water quality, which were considered by the European Directive 80/778/EEC [30] and the OECD [31] and USEPA [32] guidelines for human consumption.

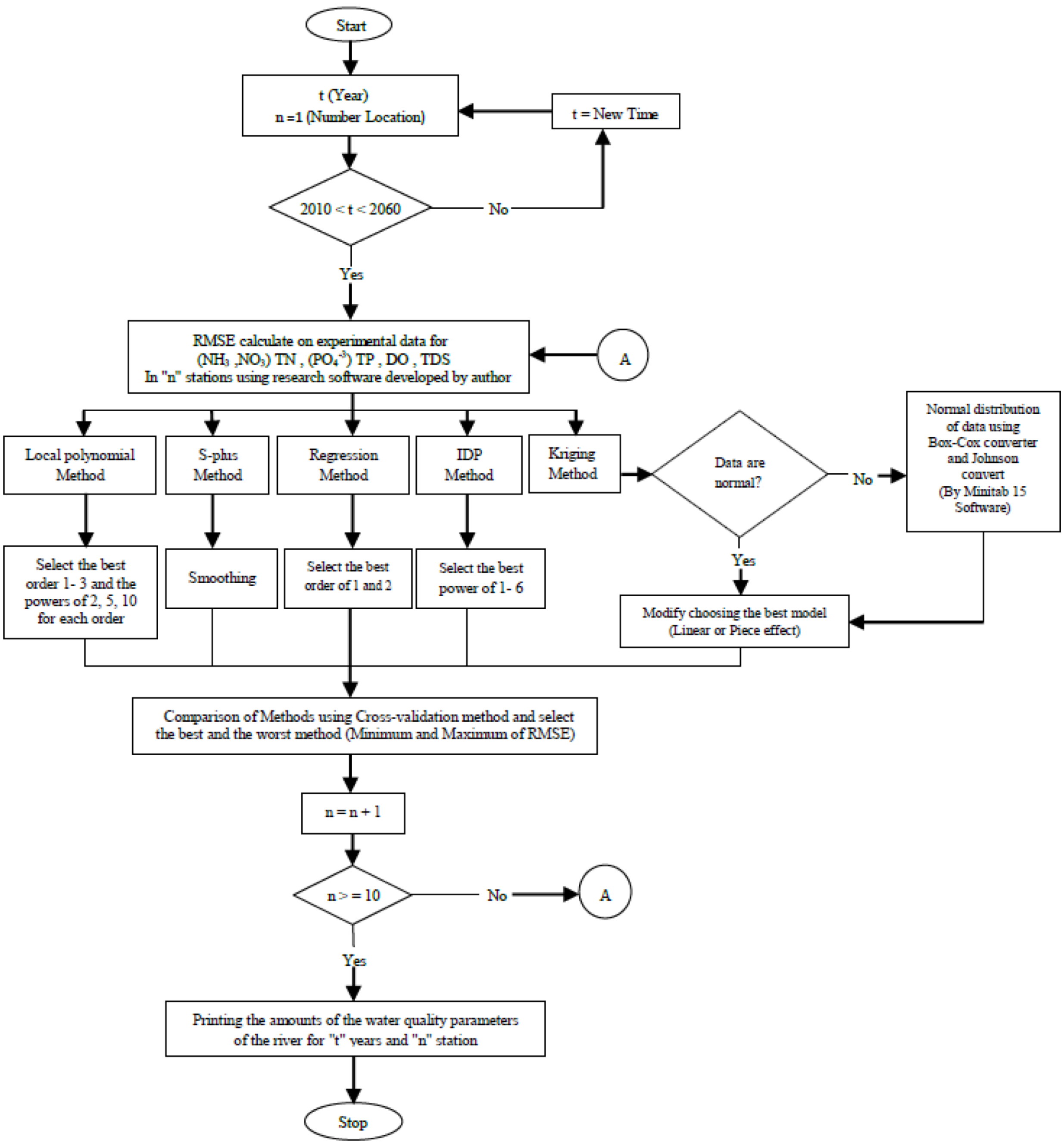


Fig. 4. Flowchart of water quality model for estimating the nutrient.

Table 2
Concentration of some quality parameters of water in the estuary of the Peer-bazar River in 2014–2015

No. Station	PO_3 (mg/l) Mean ± SD	NH_4 (mg/l) Mean ± SD	NO_2 (mg/l) Mean ± SD	NO_3 (mg/l) Mean ± SD	DO (mg/l) Mean ± SD	EC (µmho/cm) Mean ± SD	TDS (mg/l) Mean ± SD
1	0.56 ± 0.277	1.611 ± 0.361	0.020 ± 0.011	2.341 ± 0.480	6.03 ± 1.89	1025 ± 516	1138 ± 624
2	0.60 ± 0.370	2.243 ± 0.826	0.037 ± 0.033	2.390 ± 0.087	**2.34 ± 3.53**	1178 ± 898	1172 ± 615
3	0.48 ± 0.252	3.791 ± 0.590	0.013 ± 0.011	2.451 ± 0.224	4.39 ± 1.46	1037 ± 660	1141 ± 629
4	0.52 ± 0.349	**3.931 ± 0.623**	0.033 ± 0.031	3.892 ± 0.371	**2.42 ± 5.10**	**533 ± 174**	**864 ± 265**
5	**1.14 ± 0.686**	3.565 ± 0.399	0.032 ± 0.028	4.691 ± 0.753	5.72 ± 1.93	**414 ± 263**	**763 ± 338**
6	0.85 ± 0.359	2.682 ± 0.466	**0.091 ± 0.082**	4.871 ± 0.775	3.74 ± 2.78	1034 ± 737	1116 ± 468
7	0.26 ± 0.163	1.893 ± 0.629	0.014 ± 0.006	**5.022 ± 0.489**	4.76 ± 0.38	**667 ± 249**	1016 ± 314
8	0.49 ± 0.171	1.532 ± 0.378	0.023 ± 0.019	3.232 ± 0.591	3.27 ± 3.35	969 ± 337	1197 ± 482
9	0.53 ± 0.379	2.466 ± 0.258	0.038 ± 0.035	2.030 ± 0.535	4.42 ± 2.91	827 ± 519	1244 ± 486
10	**0.99 ±0.569**	3.518 ± 0.268	0.041 ± 0.032	2.251 ± 0.328	**1.63 ± 4.05**	1010 ± 308	1029 ± 259
Average	0.64 ± 0.377	2.723 ± 0.780	0.034 ± 0.029	3.344 ± 0.464	3.87 ± 2.50	1129 ± 778	1068 ± 411
Guide level	0.01*	**–0.05*0.05	Absence**	(25–42) **			<450***
Max	0.1*	0.1*–0.5**	0.1**	50**			<850***

* - OECD (1982)
- ** 80/778/EEC
- *** USEPA (1988)

Table 3
Mean concentration of total nitrogen (mg/L) in different seasons and points of the Peer-bazar River during 2014–2015

Sampling points / Seasons	1	2	3	4	5	6	7	8	9	10	Average (In Seasons)
Spring	0.735	1.09	1.371	0.622	0.69	0.688	1.175	1.102	1.044	1.303	0.982
Summer	0.11	0.303	0.592	0.223	1.151	0.178	0.142	0.216	1.047	0.593	0.456
Fall	0.101	0.088	0.16	0.096	0.079	0.068	0.47	0.075	1.068	0.091	0.230
Winter	0.422	0.334	0.291	0.819	0.791	0.742	0.727	0.704	1.328	1.814	0.797
Average (In Sampling Po.)	**0.342**	**0.454**	**0.603**	**0.440**	**0.678**	**0.419**	**0.628**	**0.524**	**1.122**	**0.950**	**0.616**

Table 4
Mean concentration of total phosphorus (mg/L) in different seasons and points of the Peer-bazar River during 2014–2015

Sampling points / Seasons	1	2	3	4	5	6	7	8	9	10	Average (In Seasons)
Spring	0.471	0.706	0.532	0.588	0.259	0.26	0.241	0.698	0.571	0.966	0.529
Summer	0.227	0.28	0.156	0.077	0.104	0.085	0.139	0.185	0.572	0.532	0.236
Fall	0.062	0.104	0.05	0.217	0.041	0.054	0.063	0.052	0.538	0.062	0.124
Winter	0.250	0.153	0.264	0.305	0.290	0.283	0.312	0.158	0.622	1.486	0.412
Average (In Sampling Po.)	**0.252**	**0.311**	**0.251**	**0.297**	**0.173**	**0.170**	**0.189**	**0.273**	**0.576**	**0.761**	**0.325**

Tables 3 and 4 show the mean concentration of total nitrogen and phosphorus in different points and seasons in the study region.

Concentration of each simulated parameters was compared with the measurements made in laboratory for calibration and estimation of the simulator. Comparison between the results (Figs. 5–9) indicated the proper performance of reference values.

Fig. 10 shows the relationship between EC and TDS parameters.

The simulator determines direction and water flow rate. As shown by Figs. 11 and 12, it is able to draw the velocity and flow direction profiles; it can also predict the spatial and temporal distributions of concentration for each parameter appropriately. The figures show that the direction and flow rate considerably affect water quality parameters.

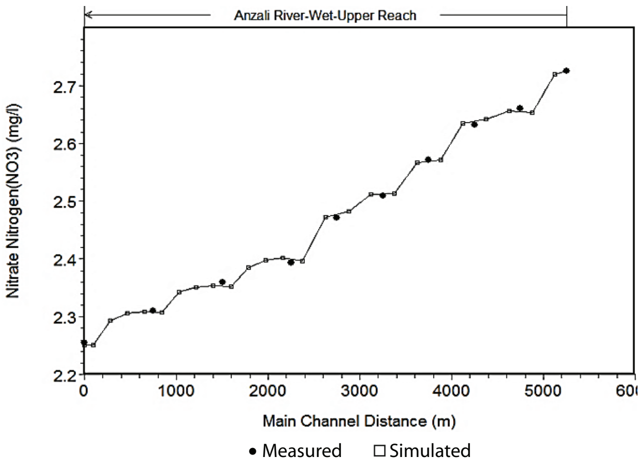


Fig. 5. Comparison between the annual changes of the calculated and measured NO_3 concentration.

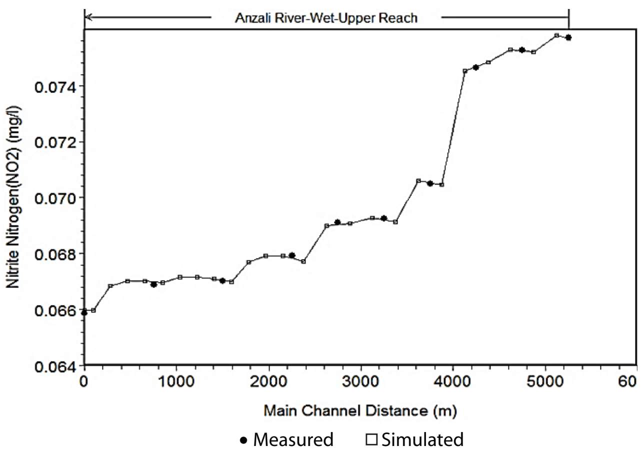


Fig. 6. Comparison between the annual changes of the calculated and measured NO_2 concentration.

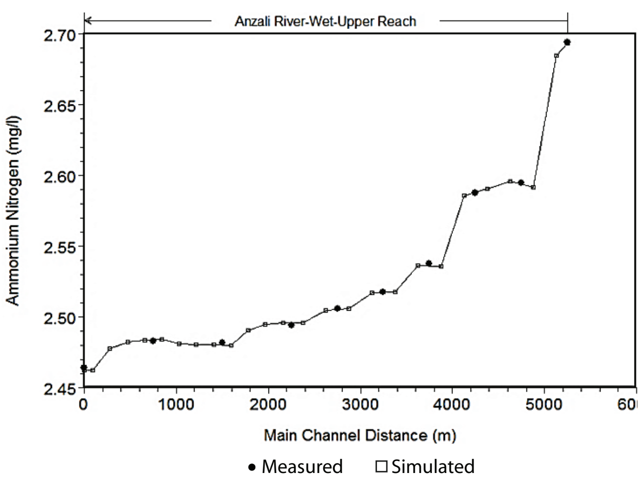


Fig. 7. Comparison between the annual changes of the calculated and measured NH_4 concentration.

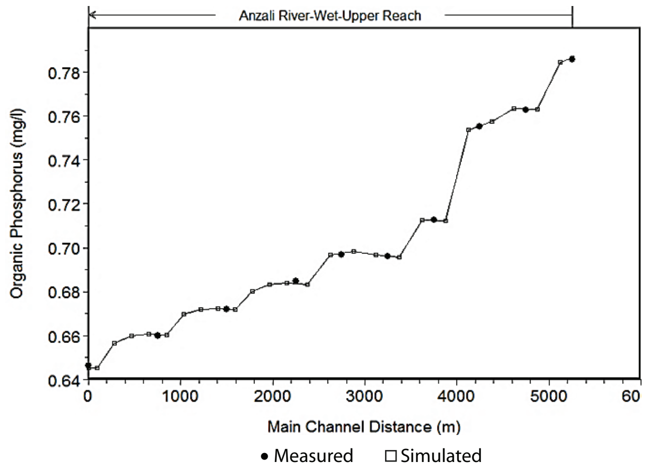


Fig. 8. Comparison between the annual changes of the calculated and measured PO_4 concentration.

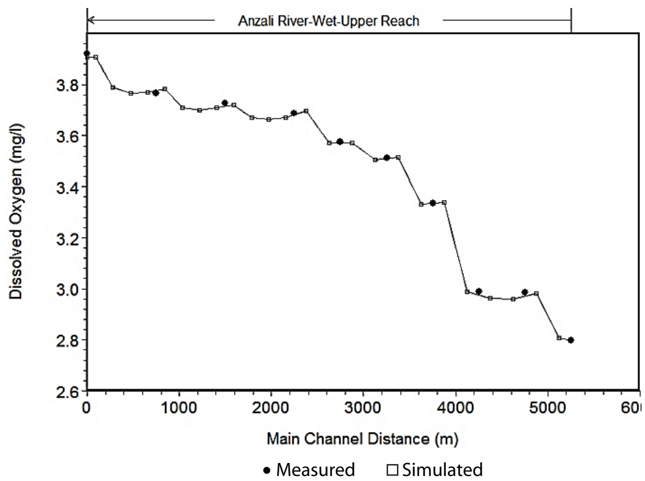


Fig. 9. Comparison between the annual changes of the calculated and measured DO.

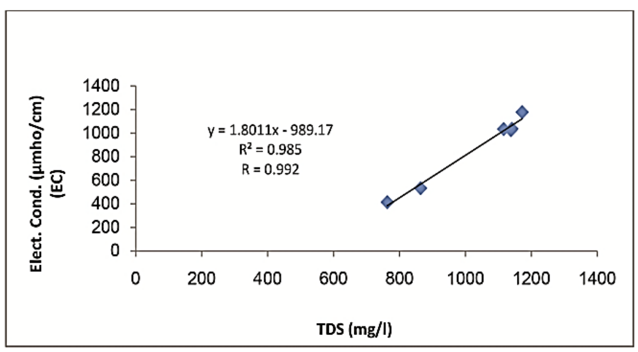


Fig. 10. Linear regression of EC and TDS during research (18 months).

3.1. Comparison of nitrogen compounds

Comparison of Nitrogen–Ammonium (NH_4^+–N) with maximum international rates of this substance in rivers showed that its concentration (1.532–3.931 mg/L) is

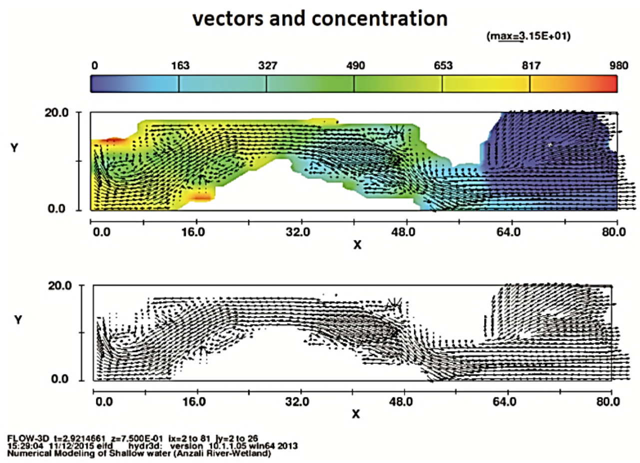


Fig. 11. Distribution of the element of horizontal velocity and direction along the waterway using the simulator.

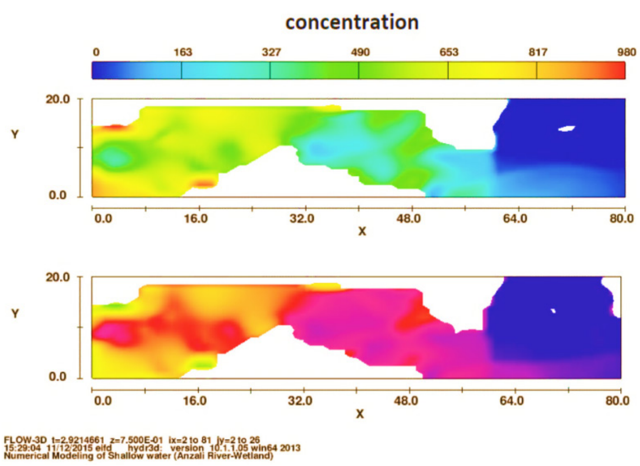


Fig. 12. Concentration of nutrients in the estuary of the Peer-bazar River in summer (upper image) in winter (lower image).

higher than the mean of permissible limit in the majority of sampling points. Excessive mean of ammonium content (2.733 mg/L) and comparing it with the other similar studies for other rivers [4,6,33] can be considered as one of the major indices of the wetland eutrophication. It can be concluded that the study wetland is subject to the advanced eutrophication conditions. The most possible reason would be the agricultural activities (discharging rice fields and the paddy fields run-off on the riverbank containing nutrients), the application of different minerals, phosphate fertilizers, and pesticides in river downstream gardens, which increase eutrophication phenomenon or the gradual aging of the wetland. With respect to the mean of pH in winter (pH = 8.29) and the rise of mean of water temperature (30.5°C), conversion of ammonium to ammonium hydroxide (NH_4OH) is probable because of the alkalinization of environment. This substance is toxic which may kill aquatics. Flowing solid sediments and increasing TDS in wetland mouth reduced wetland depth and led to premature death of the wetland [34].

Tables 1 and 2 represent that the means of water quality parameters including NO_2, NO_3, and NH_4 in different seasons are respectively within 0.014–0.091, 2.030–5.022, and 1.532–3.931 mg/L ranges. The mean of high concentration of nitrogen compounds in water samples (Figs. 5–7), which usually discharge into the river through subsurface run-off, may be derived from the decomposition of nitrogen-containing organic compounds such as protein and urea, which discharged into the environment, due to the discharge of municipal wastewater. As per the studies carried out in this research, other probable causes effective in increasing the concentrations were included the morphological changes of the bed and river path, river bank erosion, the pollution caused by solid wastes of local residents and tourists, water pollution by oil products caused by the leakage of fuel and oil used in the engine of the pumps installed at beaches, engine boats, and agricultural drainage systems. Among the studied factors, nitrate is in an appropriate condition; however, the other factors exceed the permissible range, which indicates that the river is in a polluted condition. Results showed that the total concentration of nitrogen and phosphorus in the regions with low flow rate was higher. By moving from the river upstream to the wetland entrance, nitrogen and phosphorus concentrations increased and dissolved oxygen reduced, due to the flowing of pollutants. The Increasing the concentrations of phosphorous and nitrogen was due to the flow rate reduction and increase of mud of suspended sediments into the river.

3.2. Comparison of phosphorous compounds

Algae have sufficient opportunities for consumption and accumulation of phosphorous, as water flow rate reduces in easterly of rivers and wetlands. The presence of the mean high concentration of phosphorous (Tables 2 and 4 and Fig. 8) in water samples as much as 0.124 mg/L (in autumn) and up to 0.529 mg/L (in spring) indicates water quality reduction in the water samples of the Peer-bazar river, which may accelerate nutrient and eutrophication action of region water. According to the international standards, phosphorus content between 0.01 and 0.1 mg/L is sufficient for accelerating eutrophication [35].

3.3. Total nitrogen to total phosphorous ratio

Since examining seasonal changes of surface water quality is considered as a major aspect in evaluating temporal changes of pollution of rivers due to natural and human point and non-point sources [36]. Changes distribution of total phosphorous and nitrogen concentrations during different seasons was determined based on the simulator. The mean concentration of nutrients (Tables 3 and 4) and their special and temporal distributions (Fig. 12) confirmed water quality reduction of the study region in summer (as compared with winter). It was also specified that the mean concentration of such substances in winter and spring is higher than summer and autumn. Calculations showed that the ratio of total nitrogen to total phosphorous (TP/TN) at the entrance to the wetland (downstream of the Peer-bazar River) was the maximum amount, i.e. 33.5. These values are above the permissible value of 16. According to the OECD

[31] standard, the wetlands have high tendency towards eutrophication.

Using standard error and standard deviation [Eqs. (15) and (16)], the correlation coefficient value [Eq. (17)] [37] was calculated for total phosphorus and total nitrogen in different seasons, which was between 0.87 and 0.918 (mean value = 0.894).

$$S_e = \left(\frac{1}{n-2} \sum e^2 \right)^{0.5} \tag{15}$$

$$S_y = \left\{ \frac{1}{n-1} \left[\sum y_i^2 - \frac{\left(\sum y_i \right)^2}{n} \right] \right\}^{0.5} \tag{16}$$

$$r = \left(1 - \frac{S_y^2}{S_e^2} \right)^{0.5} \tag{17}$$

The positive and high correlation between concentrations of two nutrients proved that phosphorous and nitrogen must have an identical and common source, and they mainly related to agricultural activities and rural wastewater. The correlation not only makes possible estimation of one parameter using the others, but also reduces field measurement costs. This way, the control measures on either of them will also be effective in the other. Meanwhile, coefficient of performance varies between 0.187 and 0.721, which respectively showed the optimum performance for nitrate and phosphate.

3.4. Comparison of dissolved oxygen

The relative mean reduction of dissolved oxygen (3.87 mg/L) (Fig. 9) and comparing it with other similar studies for other water sources [33,38,39], excessive growth of aquatic plants, especially Azolla, and increased plankton biomass in the wetland (water zone) confirmed that it is become eutrophic. Valuable aquatics are endangered, due the high consumption of oxygen by Azolla at nights. It is worth to mention that the concentration of dissolved oxygen during sampling was between 1.63 and 6.03 mg/L; however, oxygen-free water (0.4 mg/L) was also among the samples, which may be due to the flowing of the pollutants of agricultural non-point sources, discharging municipal wastewater (point resources) and fish ponds, and drainage of wastewater of poultry farms.

3.5. Total dissolved solids results

The data on TDS values (Table 2) show that the mean of TDS concentration exceeded 1000 mg/L in eight stations, which is considerably higher than the maximum permissible values of TDS values for such water resources as per the [32] water quality criteria. Highvalues TDS values in this research and comparing it with the earlier studies in other rivers [33,40,41] indicate that the chemical quality of the Peer-bazar River has been reduced. It is probably due to the agricultural activities (using fertilizers, toxins and pesticides in the farms around the river), deposition of sediments, aquaculture workshops, and seafood restaurants in coasts, tourism, and soil erosion.

The EC and TDS values measured for the whole year showed a robust and positive correlation between two parameters ($r = 0.95$). Regression analysis represented a linear robust relationship ($y = 1.8x - 989.2$; y = EC and x = TDS) between EC and TDS (Fig. 10). As TDS in water is a function of EC, it is possible to predict TDS concentration using EC values for reducing time and supervision costs of both parameters and propose the acceptable relationship of TDS = [(EC + 989.2)/1.8] for the wetland.

3.6. Comparison of stability and convergence

Considering the spatial and temporal variations in the equation, sensitivity analysis was carried out for Δt, Δx and Δy. The best time for simulation was obtained as 2 s. The other applied times for simulation were not suitable, due to either instability or increasing error by passing the time. Moreover, in the present simulation study, for reaching the stable conditions, *CFL* was used which led to the stable solution.

In order to obtain the suitable approximation to control numerical simulation of actual equations, the equation below was used for calculating Δt:

$$\frac{S\Delta t}{\Delta t} \leq CFL_{N_0} \tag{18}$$

With considering unequal temporal step approximation as equal, Δt was obtained via the following equation:

$$\Delta t = \frac{CFL_{N_0} \Delta x}{|S|} \tag{19}$$

where, Δx is the smallest block in the solution network, S is the velocity index and CFL_{N0} is courant number.

In addition, in this numerical simulation method, in terms of evaluating convergence, the sensitivity of mesh dimensions was investigated in longitudinal, lateral and perpendicular directions which showed that the mesh axis had the lowest sensitivity and error in perpendicular direction and the differences were similar in length steps of Δx and Δy. Results were obtained for the optimum state of mesh dimension (which is the smallest dimensions that did not show significant variations with smaller dimension) at 20, 20 and 2 cm intervals, respectively.

3. 7. Prediction and recommendations

With respect to the national and international directives and standards and according to the simulator's prediction, the region conditions will soon be worse and reach an unstable and uncontrollable critical conditions. As the changes of each water quality parameter has always been ascending (Figs. 6–9), it is predicted that the mean annual concentration of ammonium, nitrate, nitrite, phosphate, and TDS within the following ten years will be about 1.2%, 3.2%, 32%, 5%, and 7% more than the present condition. Thirty years later, the figures will be about 3.4%, 9%, 87%, 14%, and 16.5%, respectively.

It is proposed to conduct sampling study in longer intervals, to measure further rivers and quality sampling stations on direction of rivers, and to adapt them with hydrometric stations. Regarding the presence of high amount of pollutants in Peer-bazar River, sampling systems and systems measuring stability and quality of water should be installed in rivers. More importantly, water treatments for municipal wastewater and the factories near the river should be completed and developed. It is also necessary to provide a clean and healthy life for the future of the wetland using the simulator, adopting principle measures and existing potential abilities, formulating required strategies, planning, coordination, supervision and control of related institutes and organizations, and particularly applying a unique management.

4. Conclusion

This research used the software developed by the author, FLOW-3D mathematical model, and HEC-RAS for both simulation and qualitative evaluation of the Peer-bazar River. The obtained results indicated that the mean concentration of phosphorous, nitrogen, DO and TDS exceeded the permissible limits stated by the European Directive 80/778/EEC and OECD and USEPA standards. Therefore, water of the region is subject to the advanced eutrophic conditions.

In the present research, five interpolation methods namely Kriging, Inverse distance to power, Polynomial regression, Local polynomial and S-plus were applied to find the quality of river and pond water in the next decades using the developed software. The applied approaches were compared via Cross-validation method based on root-mean-square error and the best interpolation method was selected. The second-order polynomial regression (with *RMSE* of 0.2075 and 0.1475 for total nitrogen and total phosphorous, respectively) was the best model and local polynomial model with power of 10 (order of 3) was the worst method, compared to the other applied approaches.

Considering the spatial and temporal variations in the equation, sensitivity analysis was carried out for Δt, Δx and Δy. The best time for simulation was obtained as 2 s. The other applied times for simulation were not suitable, due to either instability or increasing error by passing the time. Moreover, in the present simulation study, for reaching the stable conditions, *CFL* was used which led to the stable solution.

In addition, in this numerical simulation method, in terms of evaluating convergence, the sensitivity of mesh dimensions was investigated in longitudinal, lateral and perpendicular directions which showed that the mesh axis had the lowest sensitivity and error in perpendicular direction and the differences were similar in length steps of Δx and Δy. Results were obtained for the optimum state of mesh dimension (which is the smallest dimensions that did not show significant variations with smaller dimension) at 20, 20 and 2 cm intervals, respectively.

The obtained findings of simulation predictions revealed that changes of TDS and nutrients contents will increase in the coming years and the region will reach a stable critical condition. Using regression, a relationship between EC and TDS was obtained in the next step. Comparing the results calculated by the simulator and the values measured in laboratory indicated the suitable performance of reference values.

Acknowledgements

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Supplemental

This manuscript presented the simulated results by a proposed water quality model in the case study of Iran.

My suggestion is the innovation of the study should be pointed out directly in the manuscript. Is there any development of water quality model or new finding in the case study? What is the differences between other water quality simulation studies?

The innovative points of this research that distinguish it from the other performed studies are presented as follows:

1. Up to now, the two-dimensional numerical and mathematical models of hydraulic streams discharging into the rivers for finding the concentrations of contaminants have not been studied. Therefore, this is the first study that used this model for the above mentioned purpose (Until now, for determination of contaminants in surface and river waters, the conceptual, non-dynamic and one-dimensional models have been used).
2. In addition, this model is able to exhibit animation and dynamics behavior of fluids to monitor the transport and diffusion of contaminants in water resources and find their temporal and spatial distributions at different climate conditions with high speed and accuracy. However, based on previous research, the capabilities have not been observed in previous studied models.
3. Moreover, by using the developed software prepared by the authors of this research, this is the first time that the forecasting of the quality of river water discharging into Anzali international wetland (Peer-bazar River in north of Iran) at both present and future was carried out which showed the advanced eutrophic conditions of water quality. The obtained results of forecasting by using this software revealed that the mean annual concentrations of ammonium, nitrate, nitrite, phosphate and dissolved ions in river water will be increased by 1.2, 3.2, 32, 5 and 7% in 2022, respectively. These values will be increased to 3.4, 9, 87, 14 and 16.6% in 2032, respectively, which is an innovation in water pond quality management.

QUESTION 1

More detailed information should be included to describe "Sc" in Eq. (2) because of types of nutrient parameters involved in the simulation. Is there any relation between different parameters? How could you determine different types of parameters in the model.

ANSWER 1

Since in Eq. (1), S_c has significant influence on the variety of nutritional elements in simulation process, the considered parameters of nutritional elements for S_c are reported below. The different nutritional parameters were the rate constants for physical and chemical reactions between algae, nitrogen, phosphorous, dissolved oxygen and carbonaceous biological oxygen demand (CBOD). These rate constants control S_c in equation and are also dependent on temperature [24] (In Eqs. (3) to (12), temperature dependency of each parameter related to sources/sink is marked by *. Furthermore, the name and values of different nutritional parameters and their relationship with each other are reported in Table 1).

The parameter θ is qater experimental temperature correction coefficient. This coefficient is 1.024 and 1.047 for physical and chemical reactions, respectively [25].

Source/Sinks of alive algae biomass: The water quality model can only simulate phytoplankton algae that is buoyant on the surface of water and feed from water column. The growth and respiration of algae affect the concentrations of algae, nutrient elements and dissolved oxygen in the solution. Source/Sinks of alive algae biomass can be calculated via the equation below:

$$A_{Source/\sin k} = A\mu^*_{\max}GL - A\rho^* - \frac{\sigma_1^*}{d}A \tag{3}$$

where, G is the growth limitation of algae which is obtained by nutrients formulation Leibery minimum:

$$GL = FL_{\min}(FP, FN) \tag{4}$$

where, FN is the nutrient limitation for nitrogen $\left(FN = \frac{NH_4 + NO_3}{NH_4 + NO_3 + KN}\right)$, FP is nutrient limitation for phosphorus $\left(FP = \frac{PO_4}{PO_4 + KP}\right)$ and FL is limitation for light $\left(FL = \frac{1}{\lambda h}\ln\frac{KL + 0.5}{KL + 0.5e^{-\lambda h}}\right)$ which λ is equal to $\lambda = \lambda_0 + \lambda_1\alpha_0 A + \lambda_2(\alpha_0 A)^{\frac{2}{3}}$.

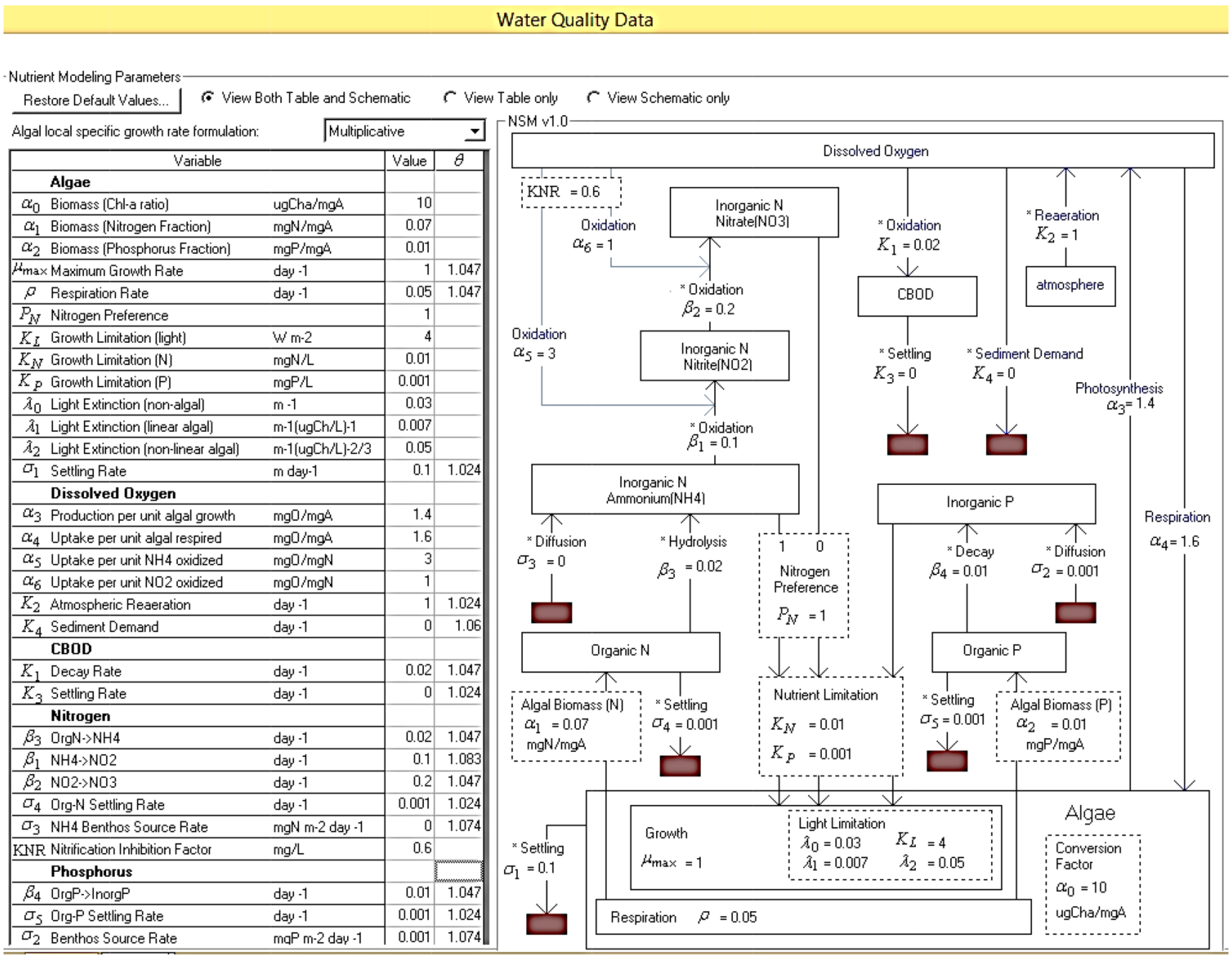
Sources/sinks of dissolved organic nitrogen: Various forms nitrogen such as $N–NH_3$, $N–NO_3$, $N–NO_2$ and organic nitrogen are present in the river water. The only internal source of organic nitrogen in the model is the algae respiration. The sinks of organic nitrogen are sedimentaion and hydrolysis for production of ammonia nitrogen. The sources/sink of organic nitrogen are as follows:

$$OrgN_{Source/\sin k} = \alpha_1\rho^* A - \beta_3^* OrgN - \sigma_4^* OrgN \tag{5}$$

Sources/sinks of ammonia nitrogen: The internal sources of ammonia nitrogen are organic nitrogen hydrolysis and dispersion from benthos. Their internal consumptions are oxidation of ammonium to nitrate and application by algae. Sources/sinks of ammonia nitrogen are calculated via the following equation:

$$NH_{4Source/\sin k} = \beta_3^* OrgNA + \frac{\sigma_3^*}{h} - \beta_1^*(1 - \exp^{-KNR-DO})NH_4 - F_1\alpha_1\mu A \tag{6}$$

Table 1
The features and relationship between different parameters of nutritional parameters in water quality model



Variable		Value	θ
Algae			
α_0 Biomass (Chl-a ratio)	ugCha/mgA	10	
α_1 Biomass (Nitrogen Fraction)	mgN/mgA	0.07	
α_2 Biomass (Phosphorus Fraction)	mgP/mgA	0.01	
μ_{max} Maximum Growth Rate	day -1	1	1.047
ρ Respiration Rate	day -1	0.05	1.047
P_N Nitrogen Preference		1	
K_L Growth Limitation (light)	W m-2	4	
K_N Growth Limitation (N)	mgN/L	0.01	
K_P Growth Limitation (P)	mgP/L	0.001	
λ_0 Light Extinction (non-algal)	m -1	0.03	
λ_1 Light Extinction (linear algal)	m-1(ugCh/L)-1	0.007	
λ_2 Light Extinction (non-linear algal)	m-1(ugCh/L)-2/3	0.05	
σ_1 Settling Rate	m day-1	0.1	1.024
Dissolved Oxygen			
α_3 Production per unit algal growth	mgO/mgA	1.4	
α_4 Uptake per unit algal respired	mgO/mgA	1.6	
α_5 Uptake per unit NH4 oxidized	mgO/mgN	3	
α_6 Uptake per unit NO2 oxidized	mgO/mgN	1	
K_2 Atmospheric Reaeration	day -1	1	1.024
K_4 Sediment Demand	day -1	0	1.06
CBOD			
K_1 Decay Rate	day -1	0.02	1.047
K_3 Settling Rate	day -1	0	1.024
Nitrogen			
β_3 OrgN->NH4	day -1	0.02	1.047
β_1 NH4->NO2	day -1	0.1	1.083
β_2 NO2->NO3	day -1	0.2	1.047
σ_4 Org-N Settling Rate	day -1	0.001	1.024
σ_3 NH4 Benthos Source Rate	mgN m-2 day -1	0	1.074
KNR Nitrification Inhibition Factor	mg/L	0.6	
Phosphorus			
β_4 OrgP->InorgP	day -1	0.01	1.047
σ_5 Org-P Settling Rate	day -1	0.001	1.024
σ_2 Benthos Source Rate	mgP m-2 day -1	0.001	1.074

where, F_1 is part of adsorbed ammonium by algae and its amount is equal $F_1 = \frac{P_N NH_4}{P_N NH_4 + (1-P_N)NO_3}$

Sources/sinks of nitrite nitrogen (NO_2): The major source of nitrite is the oxidation of ammonium to nitrite. The only sink of nitrite is its oxidation to nitrate. Sources/sinks of nitrite nitrogen can be determined via the equation below:

$$NO_{2Source/\sin k} = \beta_1^*(1-\exp^{-KNR.DO})NH_4 - \beta_2^*(1-\exp^{-KNR.DO})NO_2 \quad (7)$$

Sources/sinks of nitrate nitrogen (NO_3): The only source of nitrite nitrogen consumption is the oxidation of nitrite to nitrate. Furthermore, the only sink of nitrite nitrogen is its consumption by algae. Sources/sinks of nitrate nitrogen are determined using the following equation:

$$NO_{3Source/\sin k} = \beta_2^*(1-\exp^{-KNR.DO})NO_2 - (1-F_1)\alpha_1\mu A \quad (8)$$

Sources/sinks of organic phosphorous: The only source of nitrite nitrogen consumption is the algae respiration. The internal consumptions of organic phosphorous are phosphorous degradation for orthophosphate production and sedimentation. Equation below is used for finding Sources/sinks of organic phosphorous as follows:

$$OrgP_{Source/\sin k} = \alpha_2\rho^* A - \beta_4^* OrgP - \sigma_5^* OrgP \quad (9)$$

Sources/sinks of orthophosphate: Two important sources are reported for dissolved orthophosphate. One of them is orthophosphate degradation and another is its dispersion from benthos. The only consumption source of orthophosphate is its adsorption by algae. The following equation is applied for finding the Sources/sinks of orthophosphate:

$$PO_{4Source/\sin k} = \beta_4 OrgP + \frac{\sigma_2^*}{d} - \alpha_2\mu A \quad (10)$$

Sources/sinks of carbonaceous biological oxygen demand (CBOD): The sinks of this parameter are sedimentation and degradation with oxidation which are obtained using equation 11. But, the effect of carbon and silica cycles on this factor was overlooked, due to the low concentration of this material.

$$CBOD = -K_1CBOD - K_2CBOD \tag{11}$$

Sources/sinks of dissolved oxygen (DO): The sources of dissolved oxygen are atmospheric aeration and photosynthesis of algae. However, DO sinks are algae respiration, sediment oxygen demand, carbonaceous biological oxygen demand (CBOD) and oxidation ammonium and nitrite. Sources/sinks of dissolved oxygen are determined as follows:

$$DO_{Source/\sin k} = K_2^*(O_{sat} - DO)A(\alpha_3\mu - \alpha_4\rho) - K_1CBOD - \frac{K_4}{h} - \alpha_5\beta_1NH_4 - \alpha_6\beta_2NO_2 \tag{12}$$

QUESTION 2

Which parameter was used to understand the influence of climate changes on river flow and water quality.

ANSWER 2

In order to evaluate the effect of climate conditions on water flood and quality, several meteorology data related to climatic parameters like precipitation in catchment, air temperature and acloud were applied in model. Based on the low distance between Peer-bazar river and synoptic station of Anzali port, the obtained data of 2000–2010 were applied. Mean annual precipitation (MNP) in this station is 1857 mm which the minimum and maximum MNP are 45.6 mm (in July) and 335.1 mm (in October), respectively. Mean air temperature (MAT) is 16.2 ºC which the minimum and maximum MAT are 7.3ºC (in February) and 29.9ºC (in July), respectively. Since during 10 months of the year the weather was cloudy, 0.9 was used as an acloud coefficient in model (0.1 is for sunny weather condition). Among the other climatic conditions, atmospheric pressure, steam pressure, speed of wind and humidity were overlooked, due to either their small effect or lack of information.

QUESTION 3

In the manuscript, One-dimensional flows were simulated by HEC-RAS model, and 2D flow were simulated by FLOW-3D model. Which parts of river was simulated as one dimensional flow and which parts of river or wetland was simulated as 2D flow? and which methods were used to connect 1D and 2D or ever 3D model in the study.

ANSWER 3

Since the study area was Peer-bazer River estuaries between Ghalam Goodeh and Sooser downstream, one and two-dimensional flows were simulated using HEC-RAS and Flow-3D software, respectively. In other words, all parts study region, which was explained in paragraph 2.2, were simulated using one-dimensional and two-dimensional simulators [29].

In this regards, a one-dimensional model was prepared using HEC-RAC software and the results were applied in the *text* format as an input information for preparation of two-dimensional model (the one-dimensional information can be considered as the measured data of river water quality parameters). The results of two-dimensional model were revised, if necessary. For example, "flow velocity" and "water level" were revised as follows:

Modification of flow velocity and water level: According to the results of two-dimensional simulation, the passed flow and mean of water level of calculated section were compared with the obtained similar parameters from one-dimensional model.

$$Q_{i_{1D}} = \sum_{j=1}^{j_{y_{\max}}} Q_{i,j_{2D}}$$

$$H_{i_{1D}} = \frac{1}{j_{y_{\max}}} \sum_{j=1}^{j_{y_{\max}}} H_{i,j_{2D}}$$

where, Q_{i1D} and H_{i1D} are respectively the input flood and water level in section i in one-dimensional model. $Q_{i,j2D}$ and H_{i1D} are input flow and water level from element j in section i in two-dimensional model, respectively and J_{ymax} is the number of elements in section i in two-dimensional model. If the differences in the amount of above equations are higher than the required accuracy, the modified values of flow velocity and water level will be solved by the equation to reach the required accuracy.

QUESTION 4

Fig. 5–Fig. 9 shows the comparison between calculated and measured water quality parameters along the channel, is there any verification for 2D flows before the simulation.

ANSWER 4

As mentioned above, one-dimensional and two-dimensional models were solved based on the above method.

QUESTION 5

In the section "3. Results and Discussion", it is only simulated results were presented, more detailed discussion are recommended for establishment of simulation model or finding in the case study before draw a conclusion.

ANSWER 5

It was revised in manuscript.

The related discussion has been mentioned in detailed in 3.1 to 3.6 sections of the manuscript. Furthermore, in the present research, five interpolation methods namely Kriging, Inverse distance to power, Polynomial regres-

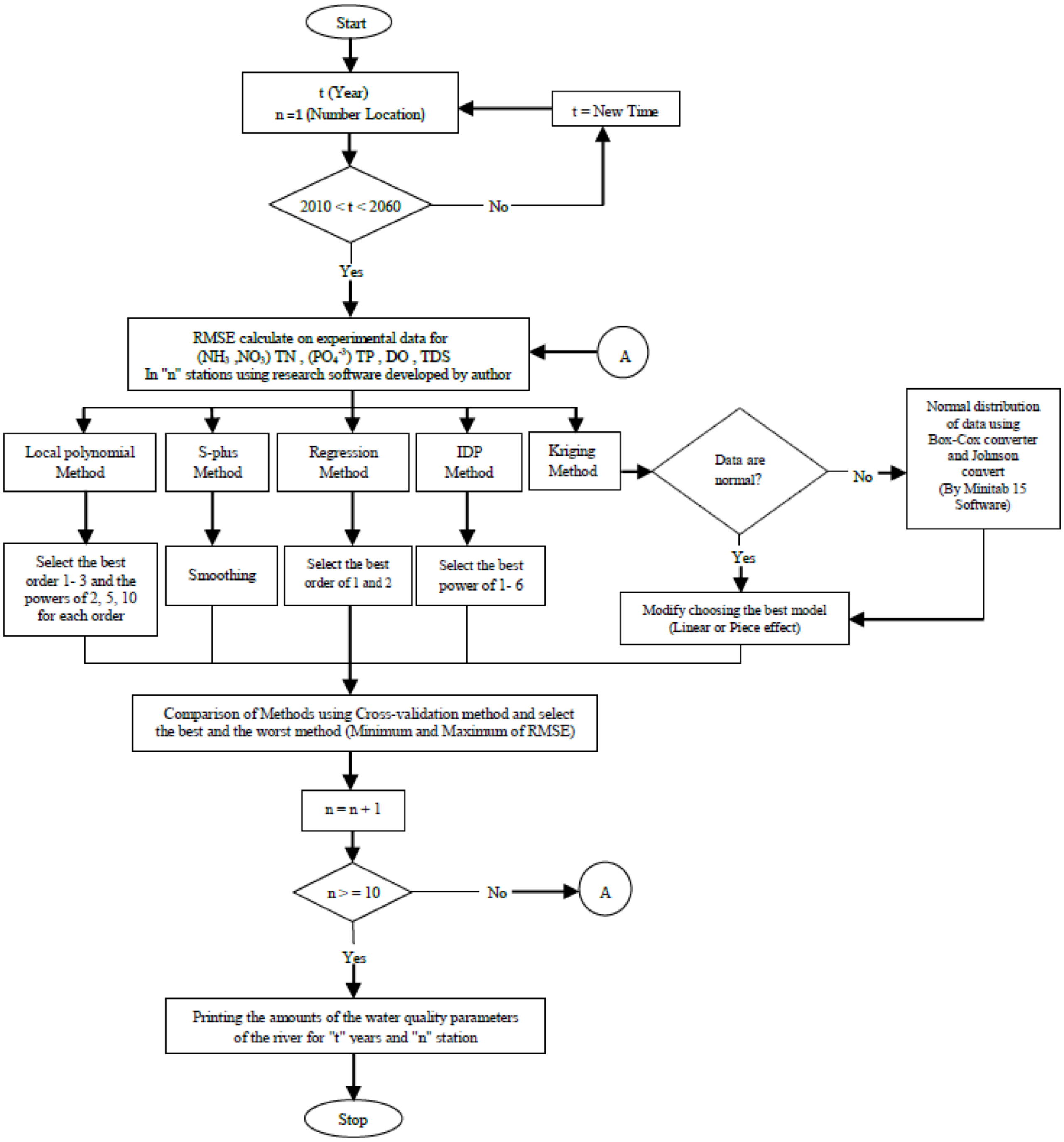


Fig. 4. Flowchart of water quality model for estimating the nutrient.

sion, Local polynomial and S-plus were applied to find the quality of river and pond water in the next decades using the developed software. The applied approaches were compared via Cross-validation method based on root-mean-square error and the best interpolation method was selected (based on Fig. 4 which was replaced with previous flowchart). The second-order polynomial regression (with *RMSE* of 0.2075 and 0.1475 for total nitrogen and total phosphorous, respectively) was the best model and local polynomial model with power of 10 (order of 3) was the worst method, compared to the other applied approaches.

Considering the spatial and temporal variations in the equation, sensitivity analysis was carried out for Δt, Δx and Δy. The best time for simulation was obtained as 2 s. The other applied times for simulation were not suitable, due to either instability or increasing error by passing the time. Moreover, in the present simulation study, for reaching the stable conditions, *CFL* was used which led to the stable solution.

In order to obtain the suitable approximation to control numerical simulation of actual equations, the equation below was used for calculating Δt:

$$\frac{S\Delta t}{\Delta t} \leq CFL_{N_0}$$

With considering unequal temporal step approximation as equal, Δt was obtained via the following equation:

$$\Delta t \frac{CFL_{N_0}\Delta x}{|S|}$$

where, Δx is the smallest block in the solution network, S is the velocity index and CFL_{N0} is courant number.

In addition, in this numerical simulation method, in terms of evaluating convergence, the sensitivity of mesh dimensions was investigated in longitudinal, lateral and perpendicular directions which showed that the mesh axis had the lowest sensitivity and error in perpendicular direction and the differences were similar in length steps of Δx and Δy. Results were obtained for the optimum state of mesh dimension (which is the smallest dimensions that did not show significant variations with smaller dimension) at 20, 20 and 2 cm intervals, respectively.