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Investigating sensitivity of flow parameters and uncertainty analysis of nutrient transport and dispersion model in shallow water. (Case study: Peer-Bazar River and Anzali Wetland)

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ABSTRACT

Accurate modeling of runoff in watersheds requires calibration and uncertainty analysis of effective flow parameters and identifying of their statistical characteristics based on inter-parameter relationships and model inputs. In this research, the transport and diffusion of pollution (nutrients) in the river were simulated through the two-dimensional finite-volume method using the shallow water equations. To numerically solve these equations, the governing equations were converted into linear equations. Uncertainty and sensitivity of the prepared pollution model were analyzed to achieve better results in estimating pollution concentrations in rivers within a reliable range. In this study, the likelihood weight (LW) method was used for each parameter in which the ratio of sensitivity and probability density function for the sets of good and bad parameters are computed. To this end, 6,000 iterations of the uncertainty domain for 3 calibration parameters of the pollution transport and dispersion model were carried out using a modification of the general likelihood uncertainty estimation (GLUE) method prepared by the authors. The three considered parameters were n (manning coefficient), S_x, and S_y (riverbed slope parameters in x and y directions) since they were more prone to measurement errors compared to the other hydraulic parameters. In the next step, the eutrophication issue and transport and diffusion of the nutrients (TDN model) in the estuaries of the Peer-Bazar River and Anzali Wetland were analyzed. A total of 1,500 simulations were considered as efficient simulations by applying the acceptable threshold values to the sum of squared errors indicator for all the simulations. The corresponded set of parameters was considered as good set parameters and the others as bad set parameters. By extracting the diagrams of the posterior probability distribution for the parameters included in the efficient simulations, parameter n with an optimal value of 0.2502 was recognized as the sensitive and influential parameter of the model. S_x and S_y with the optimal values of 0.0169 and 0.0776 were recognized as the less sensitive parameters due to their larger level of uncertainty. Assuming a confidence interval of 95% for the upper and lower bounds of uncertainty, p- and d-factors were, respectively, obtained as 0.78 and 0.73, indicating the high level of observational concentrations for the considered confidence interval. It can be concluded that the GLUE approach has been successfully applied to the TDN model. Also, the comparison of sensitivity analysis of parameters based on the LW methods and variation coefficient of parameters indicated that LW is an efficient method for sensitivity analysis of model parameters.

Keywords: Sensitivity measurement, Anzali watershed, Calibration, TDN model, GLUE algorithm

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1. Introduction

Uncertainty is an inherent, unavoidable characteristic of the modeling process which is caused by the lack of certainty and presence of errors in the model input data, parameters, and model structure [1]. Therefore, the quantification of uncertainty in the output of models is necessary to achieve reliable modeling predictions. Herewith, there are some parameters in hydraulic and hydrologic models that cannot be measured directly [2]. Estimation of hydraulic and hydrologic models parameters by various approaches and different optimization algorithms are generally error-prone, and therefore, a successful application of a hydraulic model in applied water research strongly depends on calibration and uncertainty analysis of model output. Calibration-modification and frequent changing of the number of parameters is a known issue in hydraulic and hydrologic models. Therefore, it is necessary to utilize methods for sensitivity analysis and reduction of the number of the parameter to calibrate models.

Examination and quantification of the uncertainty parameter/s, as the main objective of this study, have been mainly brought into attention in recent decades ([3–14]). Mirbagheri et al. studied water quality parameters in shallow-water problems such as rivers, reservoirs, and wetlands using Water Quality Analysis Simulation Program and MIKE families and similar models [15–24]. Herewith, several methods have been presented for the expression and analysis of uncertainty in modeling. The generalized likelihood uncertainty estimation (GLUE) method presented by Beven and Binley [25] is an important and highly applicable method competing with SUFI [26] and MCMC [27] methods as far as accuracy and ease of simulation of model uncertainty are concerned.

The reason for the broad international interest in this study, and its innovations and new findings, as well as its differences with other similar studies regarding the sensitivity analysis and uncertainties of the hydraulic models, are summarized below:

- As the innovation in this study, the emphasis has been placed on the mutual recognition of data and parameters in an uncertain state. Therefore, the study results are concerned with shallow waters, specifically rivers and wetlands, polluted with nutrients (nitrogen and phosphor in particular). Moreover, the distribution of temporal and spatial concentration for each of the mentioned parameters can be determined with high reliability at the model outputs. The reliability was validated and compared with the observational data of Homami et al. [24] and the standard models such as those proposed by Li and Duffy [6] and Baetle [28].
- In contrast to the GLUE method, which assumes the model parameters are uniformly distributed, this study employed the real (observed) distribution of parameters [24] in the hydraulic (and not hydrologic) model.
- As a reliable innovation in this study with no similar cases in the literature, the likelihood weight (LW) method was used based on the probability distribution function to evaluate and determine the sensitivity of output parameters from the GLUE uncertainty analysis for a two-dimensional (2D) pollution transport model in shallow waters. A review of the models presented in the literature reveals that no similar approach has been taken before and that studies have mostly focused on methods such as coefficient of variation, regional sensitivity analysis, sensitivity indicators, sensitivity level sampling, shuffled complex evolution and using a diagram of the posterior probability distribution of parameters. Given its relatively appropriate and accurate results, the LW method was used for this model. In the "results and discussion" section, the results from this method were compared with those of the sensitivity analysis method based on the coefficient of variations.

In general, as stated earlier, this research mainly aims at discussing the sensitivity of flow parameters as well as calibrating and analyzing the uncertainty of the simulated 2D numerical model for the transport and diffusion of nutrients (TDN model) in shallow waters (Case study: The Peer-Bazar River and Anzali Wetland) through the modified GLUE method proposed by the author.

2. Materials and methods

As mentioned in three flowcharts, clarified these steps of dispersion and transport, uncertainty identification algorithm and sensitivity analysis respectively of the model, so that these steps can be summarized from A to B and B to C and C to D (Figs. 1–3).

2.1. Governing equations

The 2D flow governing equations, which were used for predicting the concentration of the qualitative parameters of shallow water, include convection-diffusion equation (Eq. (1)) and continuity equation (Eq. (2)) as follows [29].

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

$$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} + \frac{\partial (vc)}{\partial y} = 0 \tag{2}$$

In these equations, c is a concentration of qualitative components (mg/L), u is the velocity factor along the x-axis. v is velocity component along the y-axis, t is time (day), D_x and D_y are the impact factors in longitudinal and lateral axes (in m/d).

2.2. Numerical solution of equations

The finite-volume and fractional step methods were used in this research for discontinuing and solving the governing equations. If the 2D equations of shallow waters (Eq. (1)) are integrated with control volume and the Gauss divergence theorem is used for converting surface integral to the line in the transport and dispersion (diffusion) terms, Eq. (3) will be obtained as follows:

$$\frac{\partial}{\partial t}\int_{\Omega} C d\Omega + \oint H \cdot \vec{n} dS = 0 \tag{3}$$

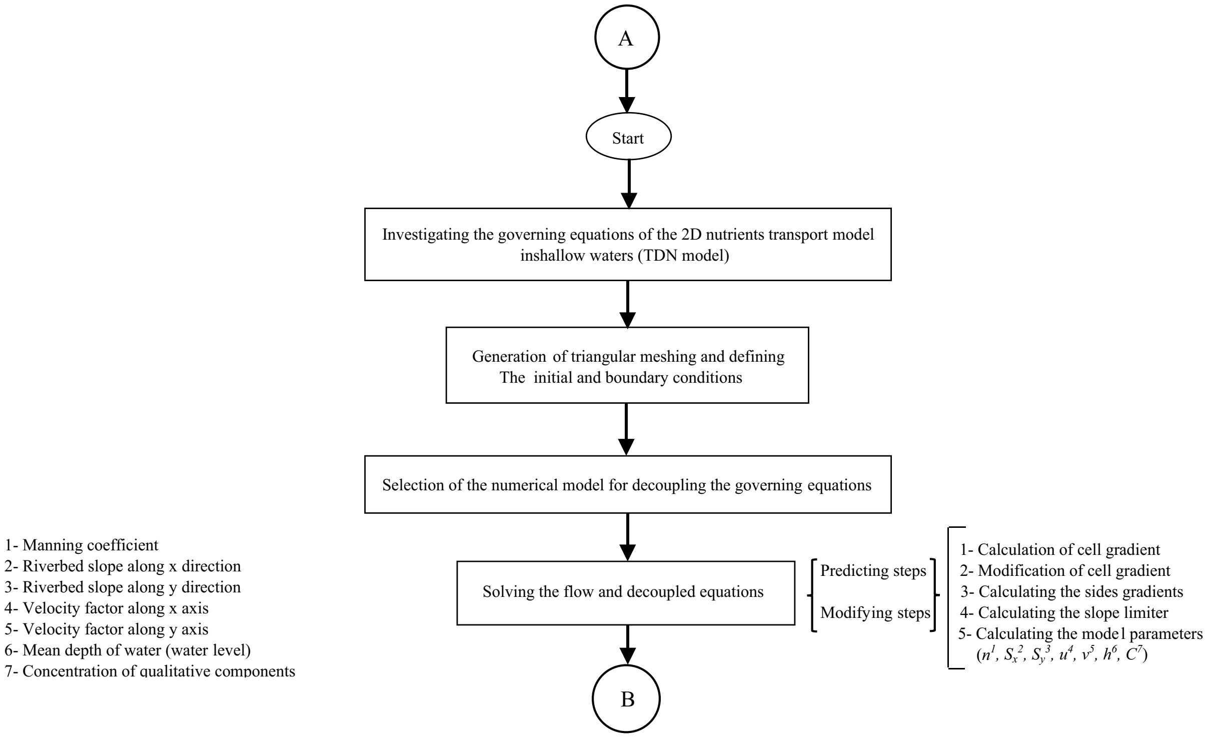

Fig. 1. Flowchart of nutrient dispersion and transport model.

where $\vec{n}$ is the perpendicular vector on the side of finite volume, Ω is the area of 2D control volume (m²) and S is in its environment (m), H is the transient flux of parameter C from each aspect of finite volume, including the two terms of transport and dispersion and is written in form of Eq. (4).

$$H = (F^C + F^D)\vec{i} + (G^C + G^D)\vec{j} \tag{4}$$

The displacement equations in the 2D space are shown in Eq. (2). The control volume used in the present research is a quadrant created by the perpendicular bisectors of corners. Considering Fig. 4, if a perpendicular plane passes on the jj_1 line, a 2D space similar to one dimensional will be created.

Ultimately, using Eq. (5), the amount of C_j^{n+1} was determined.

$$C_j^{n+1} = C_j^n - (\text{Flux}^C + \text{Flux}^D)\frac{\Delta t}{A_j} \tag{5}$$

where A_j is the area of the control volume, Δt is the time step, Flux^C and Flux^D are the parts related to the flux transient transport and dispersion terms. To use Eq. (5), the transport and dispersion terms on each edge (e) walls must be calculated as follows:

$$\text{Flux}^c = \frac{1}{2}\sum_{e=1}^{N_i}\left[\left(F_j^c + F_{j_1}^c\right)\left(y_{j_1} - y_j\right) - \left(G_j^c + G_{j_1}^c\right)\left(x_{j_1} - x_i\right)\right] \tag{6}$$

$$\text{Flux}^D = \frac{1}{2}\sum_{e=1}^{N_i}\left[\left(F_j^D + F_{j_1}^D\right)\left(y_{j_1} - y_j\right) - \left(G_j^D + G_{j_1}^D\right)\left(x_{j_1} - x_j\right)\right] \tag{7}$$

where(D_x=D_y=D): $F^C = uc$, $G^C = vc$, $F^D = -D\frac{\partial c}{\partial x}$, $G^D = -D\frac{\partial c}{\partial y}$.

2.3. Uncertainty analysis of the nutrient transport model

A problem with available results is needed to analyze the uncertainty of the nutrient transport model in the river. Therefore, a standard problem the results for which were available in the article of Homami et al. [24] was used. This problem discussed the transport and diffusion of pollution in an area with a length of 80 m and a width of 20 m in the river estuary. Fig. 5 shows the geometry used in the model and the coordinate systems.

Fig. 6 shows the model grid.

A total of 10,800 grid cells were used for the waterway, where the diffusion factor was considered to be $D_x = D_y = 0.01$. In the initial conditions, the depths of water at the bottom and the top of the river estuary were 2.5 m and 1 m, respectively. The average flow rate was 0.01 m/s and the initial pollution concentration is as follows:

$$C(x,y,0) = \begin{Bmatrix} 2 & \text{if } r \le 0.6 \\ 1 & \text{if } r > 0.6 \end{Bmatrix} \text{with} \qquad r = [(x-2)^2 + (y-1.46)^2]^{1/2} \tag{8}$$

If water depth, flow rate, and diffusion factors are assumed constant, the distribution of the pollution concentration for the contaminant (nutrients) at time t and point with the coordinates of x, y, and 0 can be obtained instantly through the following modified empirical relation [29]:

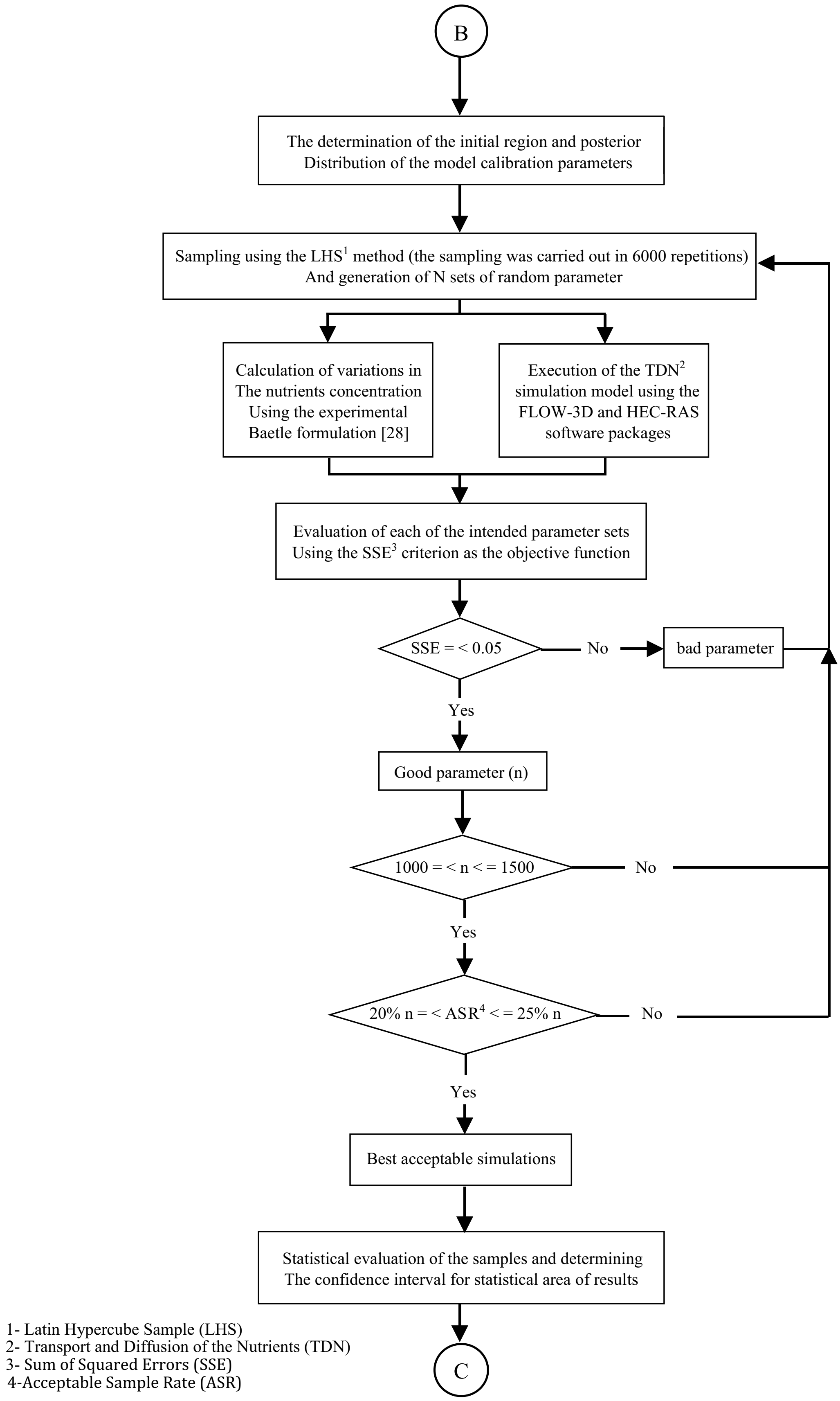

Fig. 2. Uncertainty identification algorithm for the nutrient transport model using the GLUE method (using the MATLAB software).

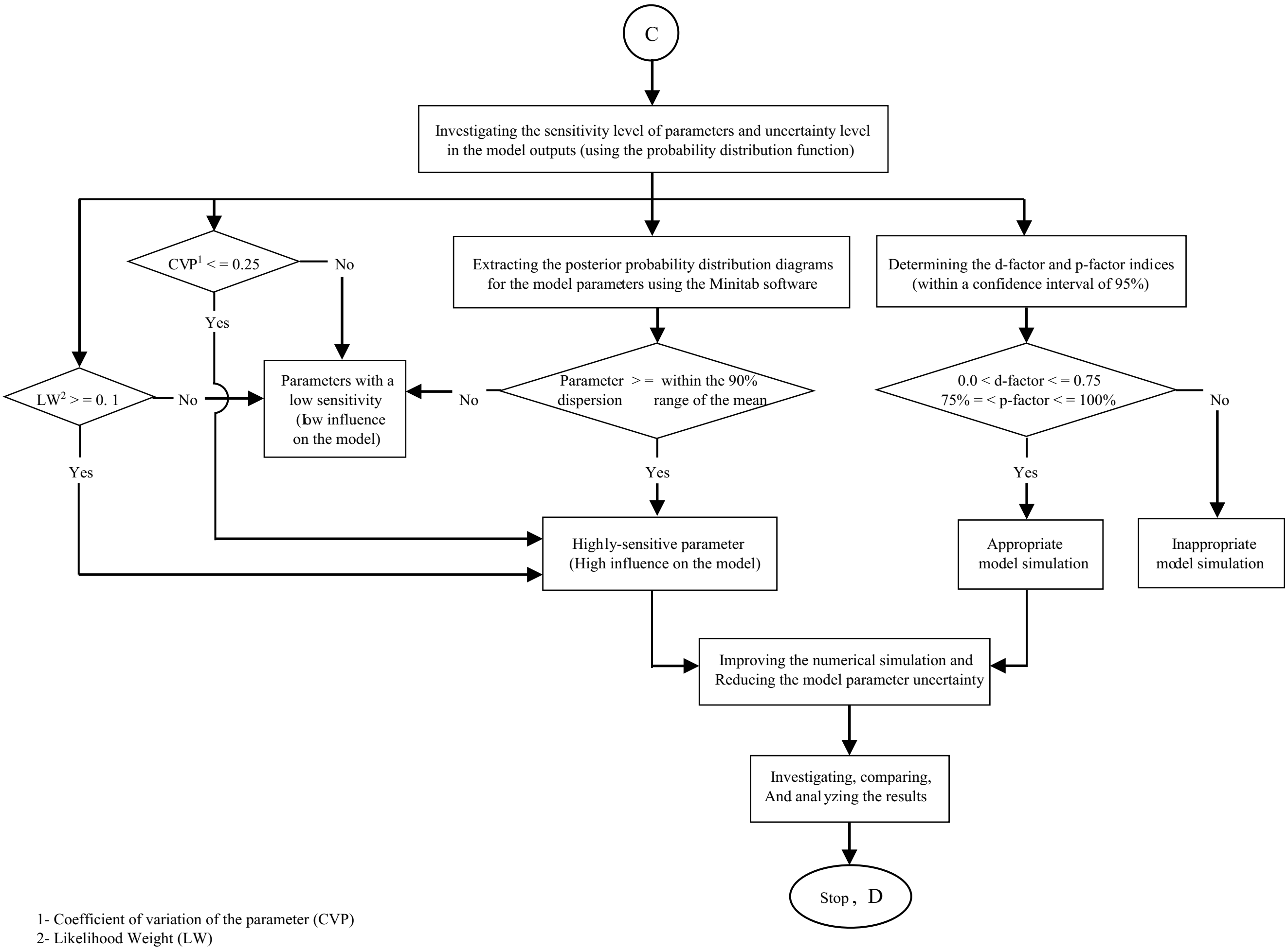

Fig. 3. Sensitivity analysis flowchart of the model parameters.

$$C(x,y,0,t) = \frac{M}{8(\pi t)^{1.5}(D_x D_y)^{0.5}} \exp\left[-\frac{(x-ut)^2}{4D_x t} - \frac{y^2}{4D_y t}\right] \quad (9)$$

where M is the mass of concentration of input nutrients with a density of 820 mg/L, which is dispersed in the environment. Other parameters are the boundary conditions of the problem geometry. The model is executed for 3 s. To the empirical relation obtained from Baetle experiments [28] and to make a more accurate comparison, the same amounts of materials with the same specifications mentioned for the numerical model were inserted in Eq. (9). The results of the empirical relation and the numerical model obtained in FLOW-3D are shown in the following figures (Figs. 7–12). The figures show pollution distribution before the uncertainty analysis of model parameters considering a constant amount for them at 0.31, 0.65, 0.97, 1.61, 1.94, and 2.59 s. As the figures show, the model simulates the dispersion and transport of materials with high accuracy.

2.4. Parameters of pollution transport model

Parameters of the pollution transport model discussed in this research were the manning coefficient (n) and the riverbed slope in x (S_x) and y (S_y) directions. Given that errors are highly likely to occur in the measurement of the riverbed slope in both directions, these parameters were considered in the uncertainty analysis. The standard problem, which was stated in the article by Homami et al. [24], was used to determine the uncertainty of the pollution transport model. For this article and similar studies such as the study of Li and Duffy [6], some intervals were considered for the calibration of parameters as shown in Table 1.

Each estimated parameter can be included in the calibration and, conversely, in case of a low sensitivity, the calibration parameter can be considered as an estimated parameter by assigning it a constant value.

2.5. Model sensitivity analysis using the LW method

In this method, the sensitivity of parameters output from the GLUE uncertainty analysis is calculated by the LWs. The uncertainty calculations for the model outputs are carried out based on the LWs of the acceptable parameters from Eq. (10) as follows:

$$\mathrm{LW}_i = \frac{L_i}{\sum_{i=1}^{N} L_i} \quad (10)$$

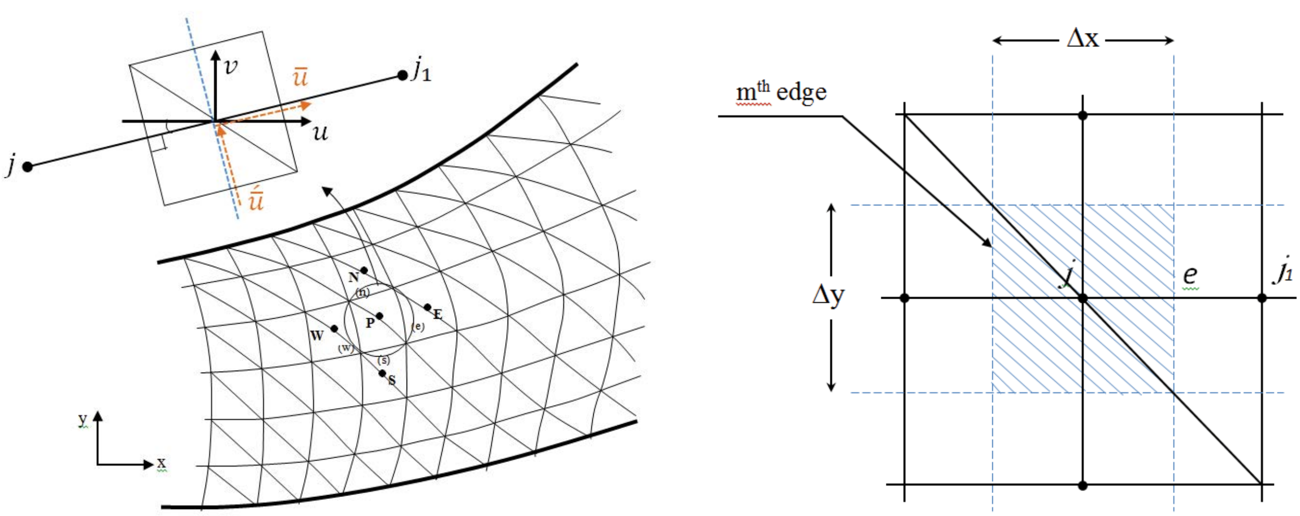

Fig. 4. Control volume around point *j* consisting of the cross section of perpendicular bisectors of the sides and definition method of velocity along each edge wall in calculative networks.

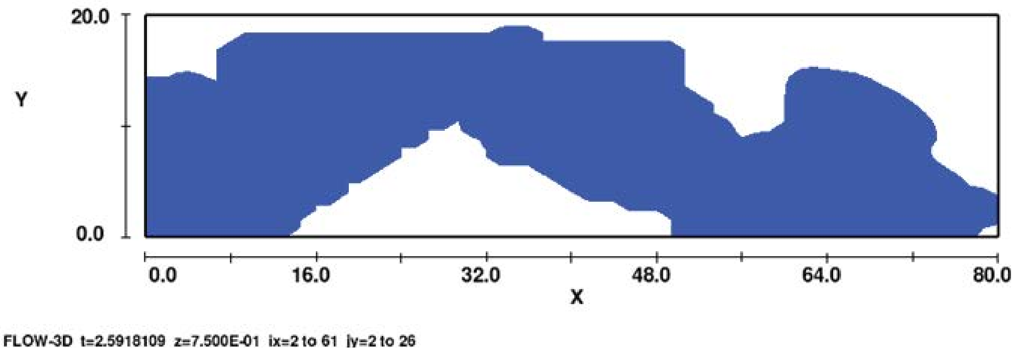

Fig. 5. Geometry used in the model.

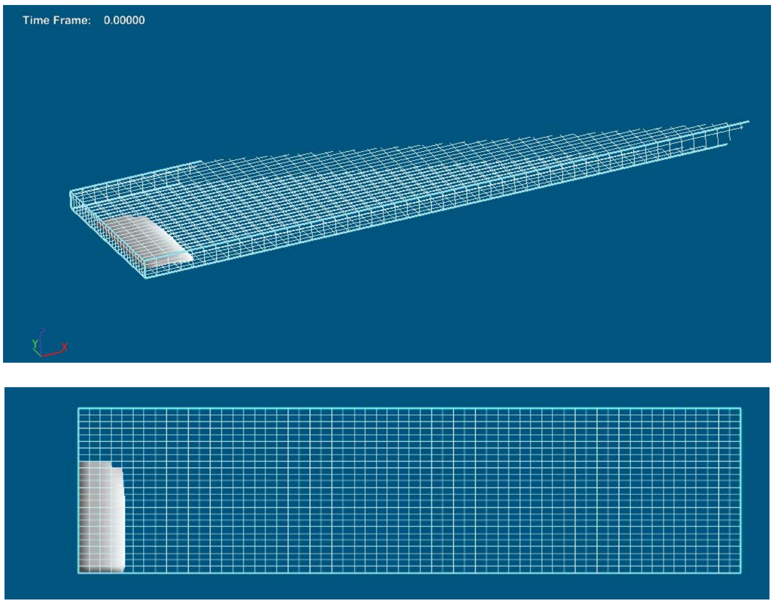

Fig. 6. Grid applied to the problem domain.

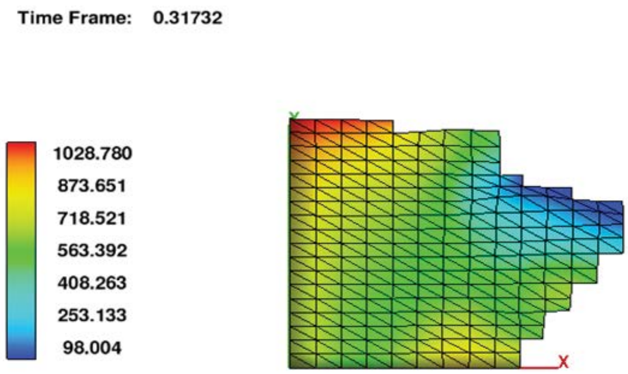

Fig. 7. Variations of pollution concentration distribution at $t = 0.31$ s.

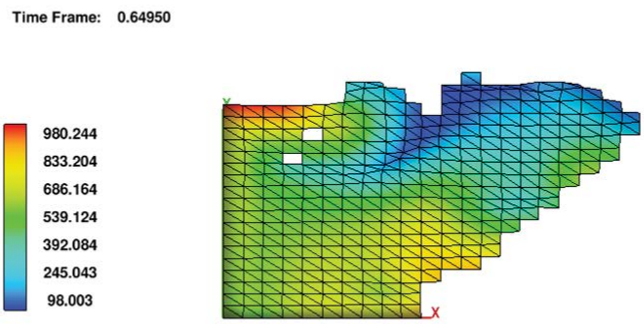

Fig. 8. Variations of pollution concentration distribution at $t = 0.65$ s.

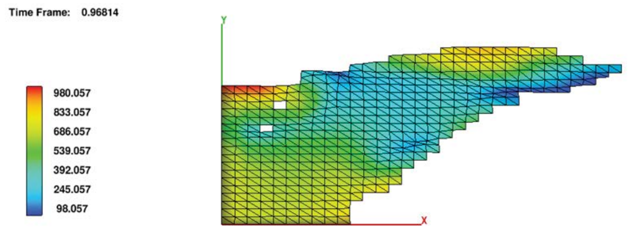

Fig. 9. Variations of pollution concentration distribution at $t = 0.97$ s.

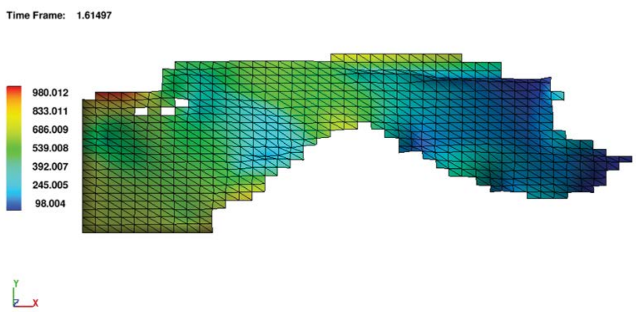

Fig. 10. Variations of pollution concentration distribution at $t = 1.61$ s.

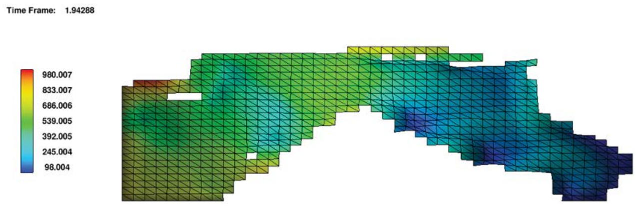

Fig. 11. Variations of pollution concentration distribution at $t = 1.94$ s.

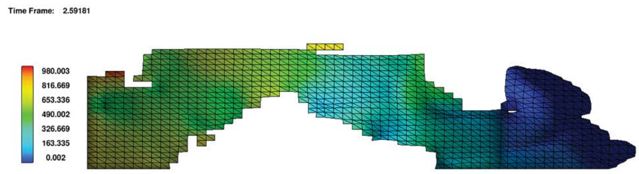

Fig. 12. Variations of pollution concentration distribution at $t = 2.59$ s.

Table 1
Sata related to the parameters of pollution transport model

Parameter	Default value	Minimum	Maximum	Estimated method
n	0.02	0.003	0.30	Calibration
S_x	0	0	0.15	Calibration
S_y	0	0	0.15	Calibration

where LW_i is the probability or LW of the i^{th} parameter set, and N is the number of acceptable parameters. Moreover, L_i is the probability function calculated from Eq. (11):

$$L_i \left(\frac{\sum_{j=1}^{n} \left(O_j - Y\left(\text{€}_i\right) \right)^2}{n = 2} \right)^{-1} \tag{11}$$

where €_i is the i^{th} parameter set, O_j is the measured values (j^{th}) parameter, $Y(\text{€}_i)$ is the model output for each parameter set, and n is the number of measured data. Larger likelihood values indicate further consistency between the simulated and real (observed) values. The sum of the LWs, which form a probability distribution function, equals 1. The obtained probability distribution is used to derive a model for the simulated output with a confidence interval of 95%.

The sensitivity analysis algorithm based on the LWs was written in MATLAB and coupled with the GLUE model which was similarly prepared in the same programming environment. The model was then executed and the outputs were analyzed as follows:

The parameters with LW > = 0.1, 0.05 < LW < 0.1, and 0.01 = < LW < 0.05 were classified as high-, average-, and low-sensitivity, respectively. Also, the parameters the LW statistic of which was not at a significance level of 95% were considered as non-sensitive parameters. Similar to the coefficient of variations method coupled with the LWs, the results indicated the suitability of the LW method.

3. Results and discussion

3.1. Model sensitivity based on the posterior probability diffusion for parameters

The three parameters of the pollution transport model were included in the GLUE algorithm to evaluate its uncertainty. Figs. 13–15 demonstrate the diagrams for the posterior functions of these parameters in the calibration step using the series of parameters generated in Minitab.

Figs. 13–15 demonstrate that the parameters with a high dispersion around the mean have a lower level of sensitivity. The higher the sensitivity of a parameter, the greater its effects on output results (simulated concentration). Therefore, the estimation of confidence bounds for pollution concentration should be performed using a higher accuracy. The dispersion of parameters in the model proves that Parameter *n*, with a biexponential posterior distribution, has a higher sensitivity and lower uncertainty. Meanwhile, S_x and S_y demonstrate a similar characteristic and are considered as parameters with a lower degree of sensitivity and higher uncertainty due to their higher dispersion of values.

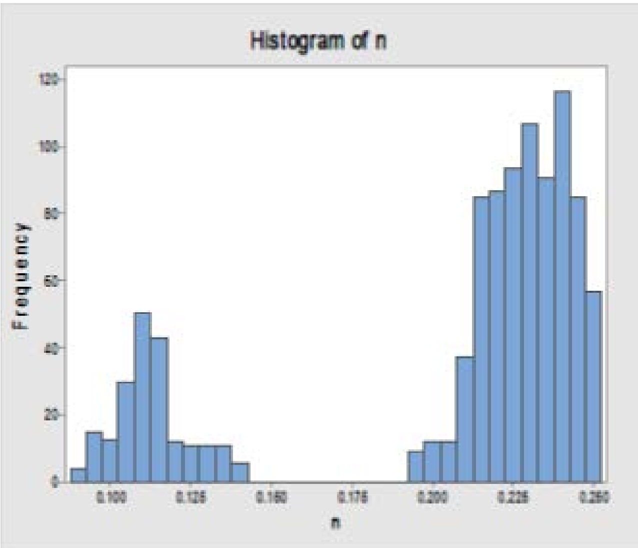

Fig. 13. Posterior probability distribution for parameter *n*.

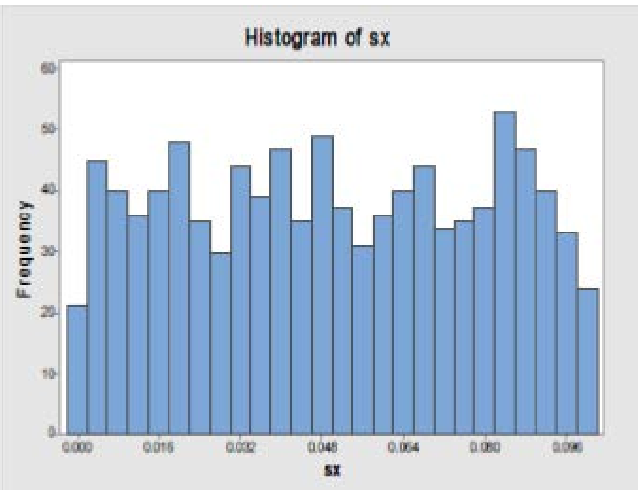

Fig. 14. Posterior probability distribution for parameter S_x.

3.2. Model sensitivity degree based on parameter variation coefficient

Conclusions can be made about the sensitivity degree of parameters by comparing some of the obtained posterior distribution statistics including the coefficient of variation of parameters. To this end, the values related to this statistic along with the mean, standard deviation (SD), LWs and the optimal values for the three considered sensitive parameters are given in Table 2 for the best simulation (the sum of squared errors). A noteworthy point to be noted is that the lower the coefficient of variations in a parameter, the higher its uncertainty and sensitivity. The uncertainty may be due to the uncertainty in input data and uncertainty in the model structure because of the simplifying assumptions considered for the real and complicated processes. Therefore, the final value of the parameter should be considered with special precision. Regarding the values of Table 2, Parameter *n* has a higher sensitivity and it cannot be replaced by a constant amount. Similar to the coefficient of variations method coupled with the LWs, the results indicated the suitability of the LW method.

3.3. Uncertainty rate criteria

The criteria used in this research for the quantification and evaluation of uncertainty rate were the *p*-factor (the percentage of the measured data within 95% confidence interval of 95 PPU) and *d*-factor (95 PPU band thickness divided by the SD of the measured data).

This way, *p*-factor and *d*-factor values closer to 100% and 0%, respectively, indicate a more appropriate simulation model. The values of the *p*-factor and *d*-factor for the calibration period were 78% and 73%, respectively. This

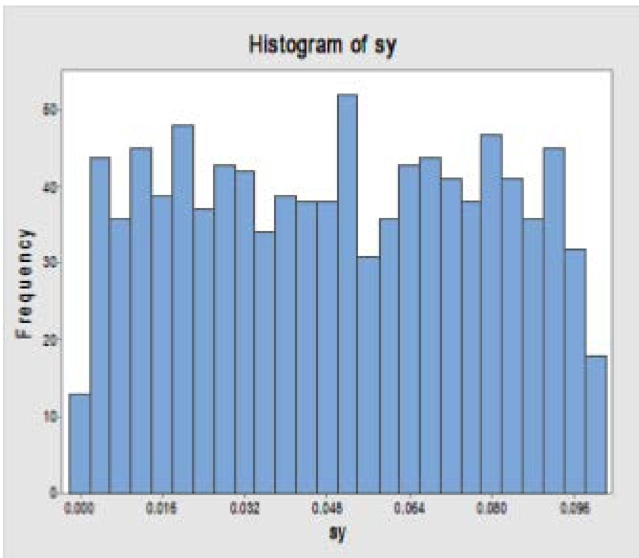

Fig. 15. Posterior probability distribution for parameter S_y.

Table 2
Optimal values for the mean, SD, LW and the percentage of variation coefficient of model parameters

Parameter	Mean	Optimal value	Standard deviation (SD)	Variation coefficient (%)	Likelihood weight (LW)	Parameter sensitivity
n	0.1994	0.2502	0.0512	24.67	0.7363	High
S_x	0.0499	0.0169	0.0301	57.33	0.0241	Low
S_y	0.0501	0.0776	0.0291	56.64	0.0189	Low

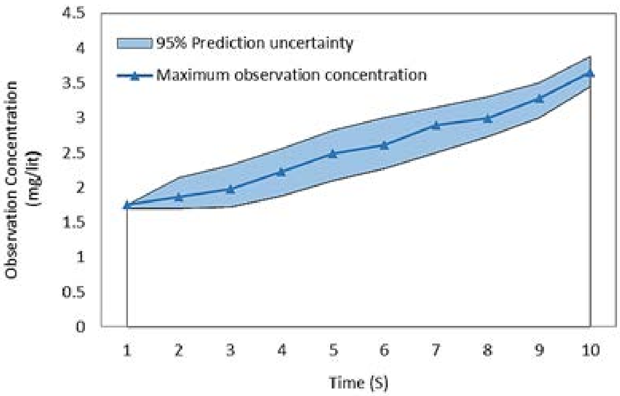

Fig. 16. The 95% interval for prediction uncertainty and maximum realistic (observational) concentration.

value for the d-factor indicates an appropriate calibration for model output. On the other hand, the p-factor, with a value of 78%, indicates an appropriate simulation given that this factor represents the percentage of observational data in a 95% interval of prediction uncertainty. Fig. 16 shows the 95% confidence interval for prediction uncertainty and the number of observations included in the interval. As shown, most of the observational data are placed within the 95% interval of prediction uncertainty, which indicates an appropriate simulation.

3.4. Employing the results and applying the model to the Peer-Bazar River and Anzali Wetland

Since the study area was Peer-Bazer River estuaries between Ghalam Goodeh and Sooser downstream, one and 2D flows were simulated using HEC-RAS and Flow-3D software, respectively and one-dimensional and 2D models were simultaneously solved.

In this regard, a one-dimensional model was prepared using HEC-RAC software and the results were applied in the text format as input information for preparation of 2D model (the one-dimensional information can be considered as the measured data of river water quality parameters). The results of the 2D model were revised, if necessary. For example, "manning roughness coefficient", "riverbed slope" and "water level" were revised as follows:

Modification of manning roughness coefficient (n), riverbed slope (S_x, S_y) and water level (H): Regarding the geometric inputs to the model, the optimal values of sensitive parameters influential on the numerical model simulating the Peer-bazar River and Anzali Wetland were input to the nutrient transport model based on the results obtained in this study (Fig. 17). The modified model was then re-executed.

According to the results of the 2D simulation, the mean water level of the calculated section was compared and modified with the obtained similar parameters from the one-dimensional model.

$$H_{i_{1D}} = \frac{1}{j_{y_{\max}}} \sum_{j=1}^{j_{y_{\max}}} H_{i,j_{2D}} \tag{12}$$

where H_{i1D} is water level in section i in the one-dimensional model. H_{i1D} is water level from element j in section i in the 2D model and $j_{y\max}$ is the number of elements in section i in 2D model. If the differences in the amount of the above equation are higher than the required accuracy, the modified value of the water level will be solved by the equation to reach the required accuracy.

4. Conclusion

Errors are inevitable parts of simulations and can usually cause problems in employing models for prediction, decision-making, and managerial assessments. Hence, the identification of uncertainties and parameter sensitivities, as an indispensable stage in deriving mathematical models, provides the designer with a broader view, allowing the decision-makers to employ the model with a deeper understanding of a phenomenon and maximize the system efficiency.

To improve the results on estimation of nutrient concentration in shallow waters and obtaining the confidence interval, the nutrient transport model was calibrated and underwent an uncertainty analysis using the modified GLUE method (presented by the authors). To this end, a total of 6,000 iterations of the uncertainty domain was performed using the GLUE uncertainty algorithm for three calibration parameters of the nutrient transport model. The standard nutrient transport and penetration problem in shallow waters were considered in this process.

The sensitive flow parameters along with uncertainty analysis of the nutrient transport model were the main results of this study, which were obtained from analyzing the outputs of the TDN model. As the important aspect of determining sensitive parameters, the extent of sensitivity of model outputs to the variations in the parameters or model structure was identified.

Results of the LW method (using the sensitivity index and probability distribution function) and through extracting the posterior distribution probability diagrams for the parameters corresponding to the efficient simulations, parameter n

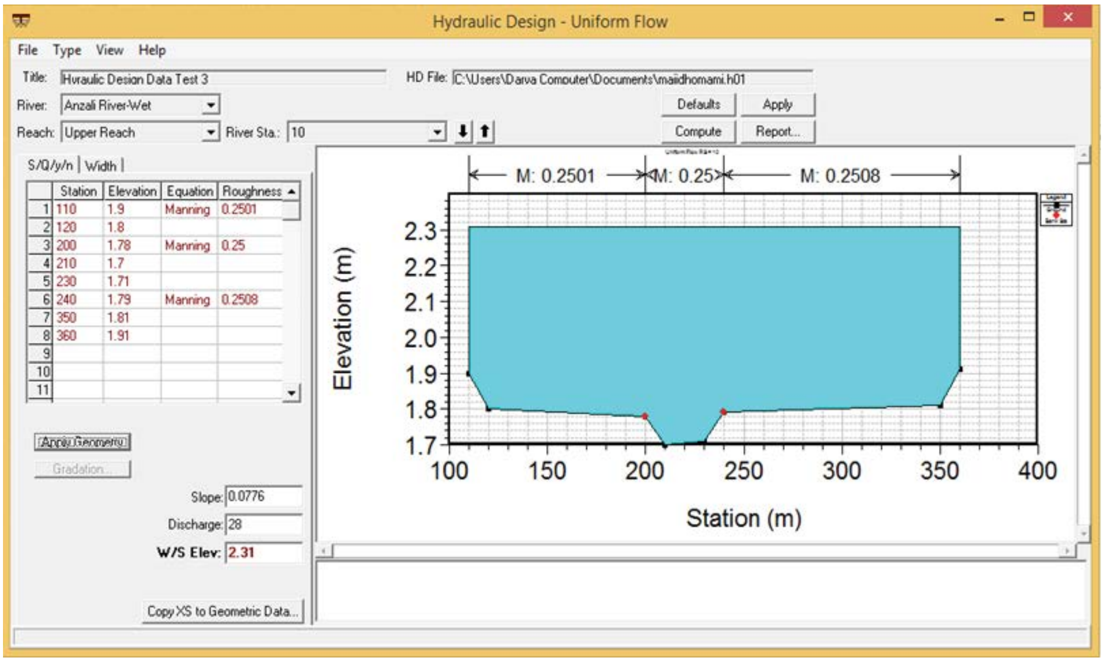

Fig. 17. Optimal value of riverbed slope input along with y direction of the model.

(manning coefficient) with the optimal value of 0.2502 was recognized as a sensitive and effective parameter. Riverbed slope parameters in x and y directions with the respective optimal values of 0.0169 and 0.0776 were recognized as the parameters with lower degrees of sensitivity due to their larger uncertainty. These results show the necessity for the calibration and uncertainty analysis of the parameters in the river pollution transport model using the 2D finite-volume method. The shape of the distribution of parameters confirmed that the model parameters might be related to the environment characteristics and geometry of the problem and its conditions.

Sensitivity analysis of the model parameters based on the LWs method and coefficient of variations method revealed the appropriate efficiency of the LW method for sensitivity analysis of the parameters in the numerical model. Hence, the LW method can be used with high reliability to analyze the sensitivity of parameters and increase the efficiency of computational fluid dynamics models.

The p-factor and d-factor were respectively 0.78 and 0.73 to the confidence interval of 95% as the top and low bounds of uncertainty, which indicated that most observational concentrations lied within the 95% confidence interval. For the framework for uncertainty analysis in the TDN model, the research results provide conditions to express model predictions in the form of a confidence interval. This is highly important in the following steps such as scenario building, managing water resources, and performing risk analysis.

To achieve better results, meshless methods, such as the meshless local Petrov-Galerkin as an efficient method for simulation of underground waters, are recommended to be used for simulation of nutrient transport in shallow waters. The model parameters are then analyzed and the results are compared with those of the LW method. Moreover, it is recommended to simultaneously simulate nutrient transport and dispersion and sediment deposition in the river.

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