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DOI 10.3390/w15020247

Publication date 2023 **Document Version** Final published version Published in

Water

Citation (APA) Kim, J., Jonoski, A., Solomatine, D. P., & Goethals, P. L. M. (2023). Water Quality Modelling for Nitrate Nitrogen Control Using HEC-RAS: Case Study of Nakdong River in South Korea. Water, 15(2), Article 247. https://doi.org/10.3390/w15020247

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Article Water Quality Modelling for Nitrate Nitrogen Control Using HEC-RAS: Case Study of Nakdong River in South Korea

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Abstract: The World Health Organization (WHO) and the U.S. Environmental Protection Agency (EPA) provide guidelines on the maximum levels of nitrate nitrogen (NO₃-N) contained in drinking water since excess nitrate ingestion may harm human health. Thus, monitoring and controlling the NO₃-N concentration is of paramount importance, especially in sources of drinking water such as the Nakdong River in South Korea. This study addresses NO₃-N pollution in the Nakdong River in South Korea, where such pollution mostly comes from diffuse sources in the catchment due to the agricultural use of fertilizers. The objective of this study is to suggest guidelines for designing strategies to control NO₃-N in this river using a process-based model developed with HEC-RAS. The model was built based on water quality parameters (water temperature, dissolved oxygen, ammonia nitrogen, etc.) related to NO₃-N dynamics incorporating hydraulic and meteorological data. This model simulated NO₃-N dynamics downstream under 55 scenarios while focusing on a section near locations of drinking water intakes. The scenarios were constructed based on variations in water quantity and quality upstream. The simulation results showed that the peak concentration of NO₃-N downstream could be directly controlled by limiting the NO₃-N concentration upstream. Additionally, control of the flow rate upstream could also lead to a reduction in the overall average concentration of NO₃-N downstream, but this predominantly occurred when the NO₃-N concentration was decreasing. In conclusion, the design and implementation of strategies for the control of NO₃-N downstream should be carried out after performing a quantitative analysis of the impact of different control measures for different downstream conditions using a water quality model.

Keywords: water quality model; HEC-RAS; nitrate nitrogen (NO₃-N); Nakdong River; water quantity; guidelines

1. Introduction

Climate change has already negatively impacted water resources in terms of quantity and quality [1]. This has prompted increasing interest in ways to effectively improve water quality, especially in rivers and surface water bodies that provide water for the public water supply. A severe reduction in water quality can pose a risk to public health by increasing human exposure to contaminated water [2]. Among the major sources of water pollution, nitrate nitrogen (NO₃-N), one of the nitrogen fractions [3], may cause specific cancers and adversely affect human reproduction when people take it in excess [4–6]. In this regard, the maximum contaminant level (MCL) of NO₃-N has been set to 10 mg L⁻¹ for drinking water by the U.S. Environmental Protection Agency (EPA). The same standard in drinking water has been applied in other countries such as South Korea [7] and Japan [8]. The European Nitrate Directive has required designating areas with surface water or groundwater whose nitrate (NO₃⁻) concentration has been more than 50 mg L⁻¹ as Nitrate Vulnerable Zones [9].



Citation: Kim, J.; Jonoski, A.; Solomatine, D.P.; Goethals, P.L.M. Water Quality Modelling for Nitrate Nitrogen Control Using HEC-RAS: Case Study of Nakdong River in South Korea. *Water* **2023**, *15*, 247. https://doi.org/10.3390/w15020247

Academic Editor: Bommanna Krishnappan

Received: 29 November 2022 Revised: 3 January 2023 Accepted: 4 January 2023 Published: 6 January 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). The 50 mg L^{-1} of NO_3^- or 11.3 mg L^{-1} (50 mg L^{-1} multiplied by 0.2258) of NO_3 -N is identical to the guideline provided by the World Health Organization (WHO) [6]. However, many studies showed that health risks could still be present despite nitrate ingestion below this MCL [6]. Thus, the water quality of reservoirs and rivers needs to be improved by controlling the concentration of this particular pollutant to make it as low as possible since reservoirs and rivers are principal sources of drinking water.

Nitrogen fractions such as NO₃-N may flow into reservoirs or rivers due to agricultural practices such as the use of nitrogen fertilizer [6]. Therefore, there is a risk of nitrate contamination in a river catchment with a lot of agricultural activities, such as the Nakdong River in South Korea [10]. Moreover, these pollutants have become water quality parameters that contribute to the complexity of water pollution [11]. NO₃-N can be not only risky as a pollutant itself, but some studies indicated NO₃-N as one of the main drivers of Harmful Algal Blooms (HABs) [12–14]. HABs have caused harm to ecology in an aquatic environment [15] and have threatened public health by producing toxic substances such as microcystin [16,17]. This is especially problematic in South Korea, where HABs have frequently created environmental problems with the four major rivers since 2012, when 16 weirs were constructed resulting in lentic water bodies in the rivers [18-21]. The specific NO₃-N concentration is hardly possible to be indicated in terms of preventing or minimizing HABs because the relationship between NO₃-N and HABs depends on other factors such as the state of water flow, site-specificity, and weather. Nevertheless, if the NO₃-N concentrations are controlled when flowing into a river or reservoir, a beneficial effect can be achieved for both the aquatic environment and public health.

A water quality model can be an effective and essential tool from the perspective of Water Quality Management (WQM). A well-developed model can help decision makers take proper precautions or emergency actions. Strategies designed with a water quality model would be more cost-effective than others, especially if they involve establishing new infrastructures or imposing government regulations [22] to control water pollution. However, success in WQM based on water quality modelling is dependent on the use of reliable data for the model setup and high performance of the developed model.

Model selection is made with consideration of various conditions including research purposes, data collection, and the required level of model performance [23]. Models (including water quality models) can be generally classified as process-based and data-driven models [24,25]. The process-based model is based on scientific theories or knowledge, while the data-driven model uses data analytics or statistical techniques. Users must select a model that meets optimum conditions after understanding its advantages and disadvantages. To achieve the desired results by developing a process-based model, the user should fully acknowledge the fate and transport of water quality parameters [26,27].

There are various modelling systems that have the capability to simulate NO₃-N dynamics in catchments and rivers—for instance, CE-QUAL-W2, SWAT, WASP7, MIKE11 [28,29], and HEC-RAS [30–35]. Developing water quality models generally requires many kinds of input variables, which is challenging for model developers [36]. Nonetheless, HEC-RAS outweighs other one-dimensional river water quality models in terms of user interface and ease of model development, although it has not been widely used compared to the others. HEC-RAS allows users to simultaneously develop a hydraulic and a water quality model [32]. In addition, HEC-RAS ensures the reproduction of river flows as realistically as possible when there are inline structures such as a weir in a river. This is because it is wellequipped with various structures for geometric data and numerous boundary condition types [32]. Several studies on water quality have recently been conducted based on these advantages of HEC-RAS. A recent study showed tangible results for nitrogen dynamics linked to unsteady flow [33], while most studies on water quality models developed with HEC-RAS were limited to the analysis of steady flow [30,31,34,35].

We aim to set out the guidelines for designing strategies to control the NO₃-N concentration using a process-based model developed with HEC-RAS for the Nakdong River. This river is an important water source for many cities located in the southeastern part of South Korea. Specifically, we first produced a model of NO₃-N dynamics for the target area of the upper Nakdong River using HEC-RAS and data from 2019 to 2020. The water quality model was developed based on the hydraulic model of unsteady flow. The downstream boundary of the model was in the vicinity of the Chilgok Weir, which is 135 km away from the upstream boundary. Second, we simulated the change in NO₃-N concentration at the location of Chilgok Weir by using the model developed in the first step. For this purpose, 55 scenarios were constructed with variation in water quantity and quality at the upstream boundary. Finally, we generated guidelines for the design of strategies to control the concentration of NO₃-N at the Chilgok Weir. These guidelines were based on the scenarios of the second step.

To the best of our knowledge, this is the first study for the Nakdong River designed to use HEC-RAS for the development of a river water quality model linked with unsteady flow. The novelty of this study is based on an in-depth analysis of the change in NO₃-N concentration in the lower reach of a river under controlled conditions of the upstream boundary such as water quantity and quality. The methodology presented in this study may also be applied for controlling HABs when linked to research that suggests NO₃-N is the main driver of HABs.

2. Materials and Methods

2.1. Study Area

The Nakdong River is the longest in South Korea, with a length of 510 km. The water quality of the Nakdong River has been a matter of concern to environmental authorities since the Nakdong River has been used as a major source for drinking water in adjacent cities [37]. The special importance of WQM in the Nakdong River has arisen from the phenol spill accident that happened in 1991 [38]. Moreover, research studies have dealt with quantitative changes in the water quality of the Nakdong River since 2012, when eight weirs were constructed [37,39,40].

We selected the upper reach of the Nakdong River for this study as shown in Figure 1. The study area covers 135 km in length from the confluence of the Nakdong River and the Banbyeoncheon River to the Chilgok Weir. From 2019 to 2020, the flow rate in this area varied from 5 to 4680 m³ s⁻¹ and the NO₃-N concentration varied from 0.240 to 3.099 mg L^{-1} .

The Andong Reservoir and the Imha Reservoir are located most upstream in the Nakdong River and the Banbyeoncheon River, respectively. The Andong Reservoir and the Imha Reservoir are connected by a water transfer tunnel for joint operation in terms of water supply, flood control, and WQM [41,42]. The Imha Dam in particular has a Selective Withdrawal Facility (SWF), so the water quality can be controlled when the water in the reservoir is released downstream [43]. Table 1 shows the details of the Andong and Imha reservoirs [44].

Table 1. Details about Andong and Imha reservoirs.

Reservoir	Andong	Imha
Area of catchment (km ²)	1584.0	1361.0
Height of dam (m)	83.0	73.0
Length of dam (m)	612.0	515.0
Normal high water level (mamsl)	160.0	163.0
Effective storage volume (10 ⁶ m ³)	1000.0	424.0

There are four weirs in the study area, including the Sangju Weir, the Nakdan Weir, the Gumi Weir, and the Chilgok Weir. Given that the intake facilities for drinking water are located between two cross sections of the Gumi Weir and the Chilgok Weir [45], the water quality for this district should be managed properly. Table 2 shows the details of four weirs [39,46]. The water level of each weir is usually maintained at each water level specified for management [47] through the operation of the gates.



Figure 1. Location of the study area.

Table 2. Details about Sangju, Nakdan, Gumi, and Chilgok weirs.

Weir	Sangju	Nakdan	Gumi	Chilgok
Area of catchment (km ²)	7407.0	9221.0	9557.0	11,040.0
Height (m)	11.0	11.5	11.0	11.8
Length (m)	335.0	286.0	374.3	400.0
Water level for management (mamsl)	47.0	40.0	32.5	25.5
Storage volume (10 ⁶ m ³)	27.4	34.7	52.7	75.3

2.2. Model Description

We used HEC-RAS version 5.0.7 for this study. HEC-RAS has several capabilities such as analysis of steady flow and unsteady flow, simulation of sediment transport, and simulation of fate and transport of water quality parameters [32]. Of these functions, we focused on the module for the river water quality analysis, which was first added to version 4.0 in 2008. The analysis of steady or unsteady flow should precede a water quality analysis [32]. As we had to consider the operations of the four weirs, we performed the analysis of unsteady flow [48] ahead of simulating the dynamics of NO₃-N, which is an output variable for this study.

HEC-RAS allows users to build a river water quality model combined with an unsteady flow analysis with inline structures including a weir. This modelling system analyzes unsteady flow by solving the Saint-Venant equation with the implicit finite difference method. The module for analysis of unsteady flow enables the application of several boundary conditions such as stage hydrograph, flow hydrograph, lateral inflow hydrograph, elevation-controlled gates, and so forth [32]. These various boundary conditions help to replicate river flows as realistically as possible. HEC-RAS also solves the one-dimensional Advection–Dispersion equation for water quality analysis using an explicit numerical method called QUICKEST–ULTIMATE (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms–Universal Limiter for Transient Interpolation Modelling of the Advective Transport Equations) [32,49,50]. The module for water quality analysis simulates the fate and transport of water temperature, dissolved oxygen (DO), carbonaceous biochemical oxygen demand (CBOD), and nutrient components such as NO₃-N [32].

2.3. Data for HEC-RAS Model

2.3.1. Data Availability

HEC-RAS requires geometric data, parameters, hydraulic data, water quality data, and meteorological data for the development of a water quality model [32]. The geometric data include the geometry of cross sections and the inline structures such as a weir [32]. Parameters for a flow model incorporate Manning's roughness coefficients of each cross section and the status of inline structures (e.g., gate conditions at weirs) [32]. For water quality, parameters include dispersion coefficients and different coefficients controlling the rate of change of different compounds with chemical reactions [32]. Furthermore, HEC-RAS needs hydraulic data such as flow rate, water quality data such as water temperature and concentrations of pollutants, and meteorological data such as atmospheric pressure [32]. When different nutrients are modelled (such as NO₃-N), their conversion rates (named 'pathways' in HEC-RAS) may be temperature dependent, and water temperature variations are modelled using the meteorological data [32].

The geometric data were obtained from the Basic River Plan for the Nakdong River, including Manning's roughness coefficients for cross sections (numbered in HEC-RAS as 411–689, see Figure 2) and the inline structures. The River Act of South Korea says that institutions for river management should make a ten-year plan for river management called the Basic River Plan and confirm its validity every five years if necessary [51]. The Basic River Plan for the Nakdong River was made in 2013.



Figure 2. Location of the monitoring stations. (**a**) Stations for hydraulic data and two weather stations; (**b**) stations for water quality data and two weather stations.

We collected data related to water quantity, water quality, and climate from the Water Resources Management Information System, the Water Environment Information System, and the Open MET Data Portal of South Korea, respectively [52]. The Act on the Investigation, Planning, and Management of Water Resources states that the institutions dedicated to hydrological investigations have to operate information systems to efficiently manage data for water resources [53]. The Ministry of Environment forms a national network to periodically monitor water quality and manages water quality data through an information system under the Water Environment Conservation Act [54]. The Korea Meteorological Administration runs an information system for meteorological data and provides the data to citizens under the Weather Act [55]. All data for the development of the HEC-RAS model are publicly available from the information systems operated under

The observational data were retrieved from 16 monitoring stations for hydraulic data, 19 monitoring stations for water quality, and two weather stations (Sangju and Gumi). The location of these stations is shown in Figure 2. The daily data are available for flow rate, water level, and climate, while water quality data is monitored almost weekly (48 or 36 times a year). We collected the data for model development in terms of the fate and transport of NO₃-N. The hydraulic data included flow rate and water level. The water quality data contained water temperature, chlorophyll a (Chl-a), dissolved oxygen demand (DO), total dissolved nitrogen (TDN), ammonia nitrogen (NH₃-N), and NO₃-N. Five types of meteorological data were collected, including atmospheric pressure, air temperature, relative humidity, solar radiation, and wind speed. Table 3 shows the mean, minimum, and maximum values of the observational data of flow rate and NO₃-N in the cross sections for model calibration (2019) and validation (2020).

Data	Cross Section		Calibration (20	19)	Validation (2020)			
(Unit)	Number	Mean	Minimum	Maximum	Mean	Minimum	Maximum	
	620	48.85	5.06	976.45	94.41	10.38	1909.73	
Flow rate	559	76.78	17.30	1675.61	173.68	18.84	2499.44	
$(m^3 s^{-1})$	505	98.87	4.27	3031.83	212.05	23.78	3632.07	
	437	116.09	24.06	4677.58	270.62	21.50	4495.12	
	658	1.313	0.679	3.038	1.445	1.055	2.453	
	620	1.398	0.240	3.058	1.547	1.095	2.512	
	559	1.750	0.807	2.872	1.844	0.900	2.924	
NO ₃ -N	517	1.688	0.651	2.935	1.840	0.993	2.858	
$(mg L^{-1})$	503	1.760	0.798	2.803	1.884	0.869	2.890	
	459	1.693	0.722	2.871	1.917	1.179	2.957	
	427	1.886	0.624	3.099	2.011	1.055	3.095	
	416	1.841	0.732	3.027	2.009	1.066	2.986	

Table 3. Mean, minimum, and maximum values of the observational data (flow rate and NO₃-N) in the cross sections for model calibration (2019) and validation (2020).

2.3.2. Data Preparation

these Acts.

We preprocessed some raw data to make them suitable for model development. The reason we needed this process is that the observational data and their frequencies do not exactly correspond to those required in the modelling system. HEC-RAS requires water temperature, algae, DO, carbonaceous biochemical oxygen demand (CBOD), dissolved organic nitrogen (DON), ammonium nitrogen (NH₄-N), nitrite nitrogen (NO₂-N), and NO₃-N [32] as water quality parameters related to NO₃-N dynamics. To address the problem of such discrepancies between the data, we interpolated the weekly data to convert them into daily data and estimated the data which are not measured—for example, algae, CBOD, and a few nitrogen components.

The following are four processes we went through for data preparation. First, the weekly data for water quality were interpolated so that they were transformed into daily

data, which is the same interval as the water level and flow data. We interpolated the water quality data by applying a step function to avoid distortion of the data variation [56]. In other words, the same values as the previous observational data were placed at daily intervals until the next data were available [57,58].

Second, we estimated the algal biomass required as input data by using the observational data of Chl-a, which is often used as a proxy index for HABs [59–61]. The concentration of Chl-a can be converted into the algal biomass with the stoichiometric ratio according to Equation (1) [33,61].

$$100.0 \text{ g Algae:} 40.0 \text{ g C:} 7.2 \text{ g N:} 1.0 \text{ g P:} (0.4-1.0) \text{ g Chl-a}$$
 (1)

where C is carbon, N is nitrogen, and P is phosphorus.

Third, a few nitrogen fractions such as NO₂-N, NH₄-N, and DON had to be estimated because they were not monitored [33]. NO₂-N was assumed to be zero since it hardly exists in rivers [62–65]. The concentrations of NH₃-N were determined by laboratory experiments using an ion analyzer [18] after converting ammonium ions (NH₄⁺) into ammonia (NH₃) by increasing the pH of samples with sodium hydroxide (NaOH). Because NH₄⁺ and NH₃ are pH-dependent, NH₃-N exists in the form of NH₄-N in most aquatic environments [66,67]. We thus replaced the data of NH₄-N required in HEC-RAS with the available data of NH₃-N. The DON concentration was calculated by subtracting the sum of NH₃-N and NO₃-N from TDN [3,63].

Lastly, we did not consider CBOD as an input variable because the module for water quality analysis in HEC-RAS calculates only losses due to oxidation and settling for CBOD [32]. We performed the sensitivity analysis on the assumption that the changes in the CBOD concentration at all the boundary conditions would not cause fluctuation in the downstream NO₃-N concentration. As a result, the assumption was valid as shown in Figure 3.



Figure 3. Graph showing the changes in the downstream NO₃-N concentration caused by changes in the CBOD concentration at all the boundary conditions.

2.4. Experimental Setup

To build a water quality model using HEC-RAS, we needed not only the geometric data but also the boundary conditions for modules for both unsteady flow and water quality [32]. We collected the geometric data by extracting the upper reach including cross sections (number 411–689) corresponding to approximately 135 km from the Basic River Plan for the Nakdong River. The daily data of flow rate were entered as boundary conditions for the cross section most upstream in addition to 10 cross sections with lateral inflows. The data of stage hydrograph was provided as a boundary condition most downstream. Regarding the four weirs included in the geometric data, we entered the data of the water levels for management as the boundary conditions of the type of elevation-controlled gate. The boundary condition of the elevation-controlled gate enables the control of the gates of the weirs in time [32]. This control of the gates was automatically taken into account in HEC-RAS based on each water level for the management (see Table 2) of the four weirs. As the boundary conditions for the water quality module, we entered the daily data interpolated from the weekly data in the cross sections where the boundary conditions for flow analysis were already given [32].

We calibrated the model parameters with data from 2019 and validated the model with data from 2020. Since the peak flow in 2019 was larger than in 2020 at the monitoring station most downstream for calibration and validation, the data from 2019 were used for calibration. The warm-up period is also necessary for model development until dynamic stability is achieved for the initial conditions [68]. Therefore, we entered the data for the warm-up period from August to December of the previous years.

The data for unsteady flow were derived from four monitoring stations for calibration and validation. For water quality analysis, we used the data from eight monitoring stations, which is twice as many stations as used for the flow analysis. The reason we used data from more stations for water quality analysis is that figuring out the fate and transport of NO₃-N is more important and complicated than flow analysis in this study. These stations were designated in consideration of the locations of the tributaries and the weirs, as shown in Figure 2, which illustrates the location of the monitoring stations. The main parameters related to NO₃-N dynamics are the conversion rates, shown in Table 4 [32], and model calibration was performed based on the default values provided in HEC-RAS. Finally, for the dispersion coefficient, we used the HEC-RAS option of automatic computation based on flow data.

 Table 4. Main parameters related to NO₃-N dynamics provided in HEC-RAS.

Parameter	Description	Default Value
Beta 3	Rate constant: DON \rightarrow NH ₄ -N	0.020
Beta 1	Rate constant: NH_4 - $N \rightarrow NO_2$ - N	0.100
Beta 2	Rate constant: NO ₂ -N \rightarrow NO ₃ -N	0.200
Sigma 4	Settling rate (DON)	0.001
KNR	Nitrification inhibition coefficient	0.600

We constructed 55 scenarios to understand how the concentration of NO₃-N downstream is changed by the variation in water quantity and quality at the upstream boundary. Three components such as flow rate, water temperature, and NO₃-N were related to these scenarios. Table 5 shows how we constructed the scenarios using these components. For example, the seventh scenario (Scenario 7) is that the flow rate of the upstream boundary increases by 50 m³ s⁻¹ for 10 days from 1 January.

Tab	le 5. 9	Scenarios	constructed	f	or an unc	lerstand	ling	of	N	Q	3-N	l d	lynamics	downst	ream
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Comp	onents *	Increment/Decrement	Period	Start Date	Scenario
Water quantity	Flow rate (m ³ s ⁻¹)	-30 -20 -10 +50 +100 +150	365 days	1 January	Scenario 1 Scenario 2 Scenario 3 Scenario 4 Scenario 5 Scenario 6
		+50 +100 +150	10 days 20 days 31 days	1 January 1 May 1 July 1 October	Scenario 7–42

Comp	onents *	Increment/Decrement	Period	Start Date	Scenario
	Water temperature (°C)	-20 -5 +10 Constant 0 Constant 15 Constant 30	365 days	1 January	Scenario 43 Scenario 44 Scenario 45 Scenario 46 Scenario 47 Scenario 48
Water quality	NO ₃ -N (mg L ⁻¹)	-1.0 -0.5 +0.5 +1.0 Constant 0.0 Constant 1.5 Constant 3.0	365 days	1 January	Scenario 49 Scenario 50 Scenario 51 Scenario 52 Scenario 53 Scenario 54 Scenario 55

Table 5. Cont.

Note: * The components belong to the boundary conditions at the upstream boundary.

These scenarios were constructed under the assumption that the water quantity and quality at the upstream boundary can be controlled. In practice, controls on the water quantity and quality can be imposed by the joint operation of the Andong and Imha reservoirs and the use of SWF installed in the Imha Dam [41–43]. The maximum increment of flow rate, 150 m³ s⁻¹, was given based on the maximum amount of water that can be released downstream via the generators of the Andong Dam and the Imha Dam. The simulations under the scenarios were carried out with data from 2018 and the developed model.

3. Results

3.1. Calibration and Validation

3.1.1. Unsteady Flow

We used Manning's roughness coefficients, listed in Table 6, for calibration of the hydraulic model. The Manning's roughness coefficient is the main parameter for calibration. We obtained the data of the coefficients from the Basic River Plan for the Nakdong River.

Table 6. Manning's roughness coefficients for the hydraulic unsteady model.

Cross Section Number	Manning Roughness Coefficient
411–467	0.024
468–672	0.026
673–689	0.028

Moriasi et al. [69] suggested the criteria of performance evaluation for watershed-scale models using Coefficient of Determination (R²), Nash Sutcliffe Efficiency (NSE), and Percent Bias (PBIAS). According to the study, model performance for flow simulations is "Good" if $0.75 < R^2 \le 0.85$, $0.70 < NSE \le 0.80$, and $\pm 5\% \le PBIAS < \pm 10\%$, while it is "Satisfactory" if $0.60 < R^2 \le 0.75$, $0.50 < NSE \le 0.70$, and $\pm 10\% \le PBIAS < \pm 15\%$. These criteria are mainly applied to watershed-scale models, but they can be used for measurement of the performance of our river model built using HEC-RAS. However, we also simultaneously employed a graphical method [69] to assess the quality of the models. Equations (2)–(4) show R², NSE, and PBIAS, respectively [69].

$$R^{2} = \left[\frac{\sum_{i=1}^{n} (O_{i} - \overline{O}) (S_{i} - \overline{S})}{\sqrt{\sum_{i=1}^{n} (O_{i} - \overline{O})^{2}} \sqrt{\sum_{i=1}^{n} (S_{i} - \overline{S})^{2}}}\right]^{2}$$
(2)

NSE =
$$1 - \frac{\sum_{i=1}^{n} (O_i - S_i)^2}{\sum_{i=1}^{n} (O_i - \overline{O})^2}$$
 (3)

$$PBIAS = \frac{\sum_{i=1}^{n} (O_i - S_i)}{\sum_{i=1}^{n} O_i} \times 100$$
(4)

where *O* is observational data and *S* is simulation result.

Unsteady flow was simulated using observational hydraulic data such as flow rate and water level as boundary conditions of HEC-RAS. As a result of both calibration and validation for unsteady flow, we carefully judged that the performance of our model was high overall in consideration of both the quantitative evaluation and the graphical method. The quantitatively measured model performance was more than "Satisfactory" except for one cross section (437), as shown in Table 7. However, the peak flows from the model simulation were not consistent with the observational data according to Figures 4 and 5, so this produced an unsatisfactory outcome of PBIAS in cross section 437. Nonetheless, since the trends in increasing flow were accurately reflected, model performance was judged as high for this unsteady flow model.

Table 7. Hydraulic model performance for unsteady flow.

Calibration/Validation	Cross Section Number	R ² NSE		PBIAS (%)	Performance	
	620	0.956	0.612	-10.3	Satisfactory	
	559	0.975	0.945	2.0	Very Good	
Calibration	505	0.967	0.962	10.5	Satisfactory	
	437	0.929	0.866	11.7	Satisfactory	
	620	0.875	0.870	-9.4	Good	
37.1.1.1.1.	559	0.948	0.937	6.5	Good	
Validation	505	0.952	0.918	9.8	Good	
	437	0.963	0.917	16.7	Not Satisfactory	

3.1.2. NO₃-N Dynamics

The water quality model for NO₃-N dynamics was developed using the hydraulic model built for unsteady flow. We simulated NO₃-N dynamics using the water quality data and the meteorological data as the boundary conditions of HEC-RAS. For calibration and validation, we used the main parameters of the model related to NO₃-N dynamics (see Table 4). One model parameter was significantly adjusted during calibration, namely Beta 3, for which a value of 0.001 was applied, while the default values were used for the other model parameters. We simulated the water quality parameters including NO₃-N by applying these model parameters. Table 8 shows the mean values of both the observational data and the simulation results for the water quality parameters from 2019 (calibration) to 2020 (validation).

Table 8. Mean values of both the observational data and the simulation results for the water quality parameters from 2019 (calibration) to 2020 (validation).

Water Quality I	Water Quality Parameter			Cross Section Number							
(Unit)		658	620	559	517	503	459	427	416		
Water temperature	Observation	15.0	14.5	16.4	16.7	15.7	16.2	17.4	15.7		
(°Č)	Simulation	13.8	12.8	12.5	12.6	12.0	12.8	12.4	12.1		
DO	Observation	10.6	10.5	10.6	11.0	10.9	10.4	10.8	10.3		
$(mg L^{-1})$	Simulation	10.6	10.6	10.8	10.8	11.0	10.8	10.9	11.1		
DON	Observation	0.483	0.424	0.418	0.428	0.359	0.375	0.425	0.379		
$(mg L^{-1})$	Simulation	0.410	0.411	0.397	0.410	0.402	0.420	0.418	0.416		

Water Quality	Parameter				Cross Secti	on Number	r		
(Un	it)	658	620	559	517	503	459	427	416
NH ₄ -N	Observation	0.062	0.048	0.055	0.045	0.053	0.050	0.077	0.091
$(mg L^{-1})$	Simulation	0.045	0.043	0.044	0.037	0.033	0.041	0.033	0.032
NO ₃ -N	Observation	1.379	1.473	1.798	1.765	1.822	1.810	1.949	1.925
$(mg L^{-1})$	Simulation	1.310	1.324	1.664	1.709	1.772	1.847	1.899	1.917



Figure 4. Hydrographs showing the difference between simulation and observation for calibration. (a) Cross section 620; (b) cross section 559; (c) cross section 505; (d) cross section 437.

Table 8. Cont.



Figure 5. Hydrographs showing the difference between simulation and observation for validation. (a) Cross section 620; (b) cross section 559; (c) cross section 505; (d) cross section 437.

We assessed the model performance for NO₃-N dynamics by adopting both the objective criteria established by Moriasi et al. [69] and the graphical method. According to Moriasi et al., model performance for nitrogen (N) is "Good" if $0.60 < R^2 \le 0.70$, $0.50 < NSE \le 0.65$, and $\pm 15\% \le PBIAS < \pm 20\%$, while it is "Satisfactory" if $0.30 < R^2 \le 0.60$, $0.35 < NSE \le 0.50$, and $\pm 20\% \le PBIAS < \pm 30\%$ at the watershed scale. The gap between the watershed-scale model and our river model was closed by simultaneously employing the graphical method in the same way as when the model performance for flow simulation was assessed.

We judged that we built a robust model for NO₃-N dynamics when carefully evaluating model performance at eight monitoring stations. Model performance for NO₃-N dynamics was more than "Satisfactory" except for one cross section (620), as shown in Table 9. Figures 6 and 7 show that NO₃-N dynamics simulated by the HEC-RAS model had a remarkably similar pattern to the observational data in eight cross sections.

Calibration/Validation	Cross Section Number	R ²	NSE	PBIAS (%)	Performance
	658	0.789	0.750	5.7	Very Good
	620	0.438	0.301	10.3	Not Satisfactory
	559	0.766	0.667	9.5	Very Good
	517	0.849	0.801	3.5	Very Good
Calibration	503	0.872	0.828	3.7	Very Good
	459	0.895	0.803	-5.0	Very Good
	427	0.816	0.732	0.5	Very Good
	416	0.852	0.777	-1.7	Very Good
	658	0.621	0.478	4.4	Satisfactory
	620	0.366	-0.155	10.0	Not Satisfactory
	559	0.494	0.442	5.7	Satisfactory
X7 1· 1 /·	517	0.652	0.640	2.8	Good
Validation	503	0.611	0.605	1.8	Good
	459	0.750	0.749	0.4	Very Good
	427	0.606	0.575	4.5	Good
	416	0.791	0.764	2.4	Very Good

Table 9. Model performance for NO₃-N.







(**d**)

Figure 6. Cont.



Figure 6. Graphs showing the difference between simulation and observation of the NO_3 -N concentration for calibration. (a) Cross section 658; (b) cross section 620; (c) cross section 559; (d) cross section 517; (e) cross section 503; (f) cross section 459; (g) cross section 427; (h) cross section 416.



Figure 7. Cont.



Figure 7. Graphs showing the difference between simulation and observation of the NO_3 -N concentration for validation. (a) Cross section 658; (b) cross section 620; (c) cross section 559; (d) cross section 517; (e) cross section 503; (f) cross section 459; (g) cross section 427; (h) cross section 416.

The model delivered high performance, especially in cross section 416, which is closest to the Chilgok Weir. The station in this cross section is located most downstream among the eight monitoring stations for calibration and validation. Cross section 416 is critically important in this study because the scenarios, provided in Table 5, were constructed for the simulation of NO₃-N dynamics in cross section 416.

3.2. *Scenario-Based* NO₃-N *Dynamics* 3.2.1. Variation in Water Quantity

Simulations under Scenarios 1–6 indicated changes in the concentration of NO_3 -N in cross section 416 caused by variations in the flow rate most upstream for the whole period (365 days), as shown in Figure 8. The black graph in Figure 8 shows the NO_3 -N concentration simulated using the observational data from 2018 as boundary conditions. We compared the other graphs, which are simulation results achieved by variation in flow rate, to the black graph.



Figure 8. Changes in the NO₃-N concentration in cross section 416 caused by variations in flow rate at the upstream boundary for 365 days. The black graph shows the NO₃-N concentration simulated using the observational data from 2018 as boundary conditions. The dispersion coefficient was automatically computed in HEC-RAS. (**a**) Changes in the NO₃-N concentration by a decrease in flow rates (Scenarios 1–3); (**b**) changes in the NO₃-N concentration by an increase in flow rates (Scenarios 4–6).

The results showed that increased flow rates at the upstream boundary led to a decrease in the NO₃-N concentrations in cross section 416. However, different aspects were explored regarding the change in the NO₃-N concentration only around July and August, as indicated by the blue ellipses in Figure 8. In other words, the peak concentration of NO₃-N increased in the blue ellipses, although the flow rate increased at the upstream boundary. This reversal was brought about when the downstream NO₃-N concentration sharply increased in the simulation result using observational data at the boundaries (black graph). Here, the increase in flow rate seems to have accelerated the dispersion of the NO₃-N concentration downstream. The acceleration in the dispersion temporarily caused a rapid increase in the NO₃-N concentration. This hypothesis can be supported by comparing Figure 8 with Figure 9, which shows the results simulated with the fixed dispersion coefficient of zero. In the blue ellipses of Figure 8, which shows the results simulated with the computed dispersion coefficients.



Figure 9. Changes in the NO₃-N concentration in cross section 416 caused by variations in flow rate at the upstream boundary for 365 days. The black graph shows the NO₃-N concentration simulated using the observational data from 2018 as boundary conditions. The dispersion coefficient was set to zero. (a) Changes in the NO₃-N concentration by a decrease in flow rates (Scenarios 1–3); (b) changes in the NO₃-N concentration by an increase in flow rates (Scenarios 4–6).

The effect of decreasing the NO₃-N concentration was more considerably exerted by an increase in the flow rate when the NO₃-N concentration downstream was decreasing than when it was increasing, as indicated by the red ellipses in Figure 8. As shown in Table 10, the flow rate that increased by 150 m³ s⁻¹ brought about a reduction effect of only 5.1%. This effect was shown when the NO₃-N concentration was increasing. On the other hand, the rate of reduction in the NO₃-N concentration was much higher (60.3%) when the NO₃-N concentration was decreasing.

Flow Rate		NO ₃ -N			
Increment (m ³ s ⁻¹)	Rate of Increment (%)	Concentration (mg L ⁻¹)	Date	Reduction in Concentration (mg L ⁻¹)	Rate of Reduction (%)
0	-	2.463	14 November	-	-
50	33.3	2.414	1 November	0.049	2.0
100	66.7	2.371	26 October	0.091	3.7
150	100.0	2.337	23 October	0.126	5.1
0	-	2.046	21 December	-	-
50	33.3	1.299	2 December	0.747	36.5
100	66.7	0.992	28 November	1.054	51.5
150	100.0	0.813	26 November	1.233	60.3

Table 10. Example, taken from the red ellipses in Figure 8b, of the change in NO₃-N concentration produced by an increase in flow rate.

Interestingly, we found that a fall in the NO₃-N concentration was not proportional to a rise in the flow rate. In Figure 8, this point is demonstrated by the unequal changes in the NO₃-N concentration corresponding to the equal-step increase in flow rate (e.g., change in concentration is high for flow variation from $0 \text{ m}^3 \text{ s}^{-1}$ to $50 \text{ m}^3 \text{ s}^{-1}$, but it is insignificant for the change from $100 \text{ m}^3 \text{ s}^{-1}$ to $150 \text{ m}^3 \text{ s}^{-1}$). In any case, ever-increasing flow rates under Scenarios 4–6 do not match the reservoir operations in practice, because this may lead to a shortage of water supply. That is why we considered Scenarios 7–42, where the flow

rates were increased at the upstream boundary temporarily instead of for the whole period (365 days).

The overall results obtained by the simulation under Scenarios 7–42 showed that the larger the flow rate, or the longer duration of the increase in flow rate, the more significant the reducing effect on the NO₃-N concentration. Nonetheless, the results showed slight differences depending on when the flow rate started to increase. For instance, in Figures 10b and 11b, it can be seen that the concentration of NO₃-N decreased compared to the black graph, depending on the amount or the duration of increased flow. On the contrary, Figures 10c and 11c show opposite results to Figures 10b and 11b. The only difference between these cases was the time when the flow rate started to increase. Figures 10b and 11b show the results achieved under the condition where the increase in flow rate began in May, when the NO₃-N concentration was falling. On the other hand, in Figures 10c and 11c, the flow rate increased at a time when the concentration of NO₃-N was markedly rising.



Figure 10. Changes in the NO₃-N concentration in cross section 416 caused by variations in flow rate (50, 100, and 150 m³ s⁻¹) at the upstream boundary for 31 days. The black graph shows the NO₃-N concentration simulated using the observational data from 2018 as boundary conditions. The change in flow rate occurred in: (a) January; (b) May; (c) July; and (d) October.



Figure 11. Changes in the NO₃-N concentration in cross section 416 caused by variations in flow rate $(100 \text{ m}^3 \text{ s}^{-1})$ at the upstream boundary for 10, 20, and 31 days. The black graph shows the NO₃-N concentration simulated using the observational data from 2018 as boundary conditions. The change in flow rate occurred in: (a) January; (b) May; (c) July; and (d) October.

In this regard, the current status of a river should be considered for decision making related to reservoir operations in terms of WQM. Specifically, decision makers should determine to what extent the flow rate released from a reservoir will be increased or decreased or when this action will be taken by considering the current status of the concentration of water pollutants. This will result in effective and efficient control of NO₃-N downstream.

3.2.2. Variation in Water Quality

We learned from Scenarios 43–48 that variations in water temperature at the upstream boundary had little impact on the NO_3 -N concentration in cross section 416, as shown in Figure 12. This phenomenon seems to emerge because the water upstream is mixed with tributaries as the water flows downstream, and the water temperature of the river reaches equilibrium. This means that there is little impact on the concentration of NO_3 -N downstream only with the change in water temperature at the upstream boundary.



Figure 12. Changes in the NO₃-N concentration in cross section 416 caused by variations in water temperature at the upstream boundary. The black graphs show results simulated using the observational data from 2018 as boundary conditions. (a) Changes in the NO₃-N concentration by a decrease or increase in water temperature (Scenarios 43–45); (b) changes in the NO₃-N concentration by constant water temperature (Scenarios 46–48).

The simulation results under Scenarios 49–55 demonstrated that a marked variation in the NO₃-N concentration occurred downstream if the concentration of NO₃-N increased or decreased at the upstream boundary, as shown in Figure 13. In other words, control over the NO₃-N concentration itself in the tributaries or the upper reaches of a river would be highly effective in controlling the concentration of NO₃-N downstream. However, the amount of variation in the downstream NO₃-N concentration may increase or decrease depending not only on the change in the upstream NO₃-N concentration but also on the current status of the river, such as flow rate and water temperature. Therefore, the control method for NO₃-N should be adopted in consideration of the current status in the target area. This sufficient consideration for the downstream status enables the establishment of effective strategies for controlling the downstream NO₃-N concentration with a water quality model.

3.3. Guidelines for Design of Strategies to Control NO₃-N Downstream

Effective strategies can be devised to control the downstream NO₃-N concentration based on the simulation results of the Scenarios of this study. Guidelines for the design of strategies can be suggested using the control methods of the flow rate or the NO₃-N concentration at the upstream boundary, which was proven effective under the Scenarios. The primary purpose of control methods should be carefully considered before employing the methods. The purpose can include control of the peak concentration or the overall average concentration of downstream NO₃-N.

Specifically, the control method of the NO₃-N concentration itself at the upstream boundary is much more practical for decreasing the highest concentration of NO₃-N downstream than a change in the flow rate at the upstream boundary. This can be demonstrated in Figure 14a, which shows conditions of both decreasing and increasing concentrations of NO₃-N in 2018 (black graph). The blue graph shows the variation in the NO₃-N concentration in cross section 416 when the NO₃-N concentration decreased by 1.0 mg L⁻¹ at the upstream boundary. The red graph shows the simulation result achieved by a flow rate increase of 150 m³ s⁻¹ at the upstream boundary. We could clearly observe that the peak concentration in the blue graph was lower than the peak in the red graph when the NO₃-N concentration was increasing (July–August 2018). Contrastingly, when the NO₃-N concentration was decreasing (May–June 2018), we could produce the effect of decreasing the downstream NO₃-N concentration by increasing the flow rate more than by reducing the NO₃-N concentration at the upstream boundary.



Figure 13. Changes in the NO₃-N concentration in cross section 416 caused by variations in the NO₃-N concentration at the upstream boundary. The black graphs show results simulated using the observational data from 2018 as boundary conditions. (a) Changes in the NO₃-N concentration by a decrease or increase in the NO₃-N concentration (Scenarios 49–52); (b) changes in the NO₃-N concentration by a constant concentration of NO₃-N (Scenarios 53–55).



Figure 14. Changes in the NO₃-N concentration in cross section 416 caused by a decrease in the NO₃-N concentration at the upstream boundary or an increase in flow rate at the upstream boundary. The black graphs show the result simulated using the observational data from 2018 as boundary conditions. (a) Changes in the NO₃-N concentration by a decrease in the NO₃-N concentration (blue graph) or an increase in flow rate (red graph); (b) changes in the NO₃-N concentration by an increase in flow rate of 100 m³ s⁻¹ (blue graph) and 150 m³ s⁻¹ (red graph) for 20 days.

Nonetheless, a large flow rate is not always fully effective. Figure 14b shows that there is a slight difference in making the downstream NO₃-N concentration decrease between an increase in flow rate of 172.8 million m³ (100 m³ s⁻¹ for 20 days, the blue graph) and of 259.2 million m³ (150 m³ s⁻¹ for 20 days, the red graph). The lowest concentrations of NO₃-N were 1.212 mg L⁻¹ (on 27 January) and 1.097 mg L⁻¹ (on 22 January) in the blue and red graphs, respectively, with a difference of only 0.115 mg L⁻¹.

4. Discussion

The simulation results showed how the downstream NO₃-N concentration would respond depending on variation in the quantity and quality of water upstream. With these results, general guidelines for strategies to control downstream NO₃-N can be suggested with the control methods for the peak concentration and the overall average concentration of NO₃-N. The peak concentration of downstream NO₃-N can be directly controlled by limiting the concentration of NO₃-N in the tributaries or the upper reaches of a river. Control of the upstream flow rate is a viable strategy in terms of control over the overall average concentration of downstream NO₃-N when its concentration is decreasing. Notably, the strategy related to water quantity can be effectively implemented by deciding how much the flow rate should be increased after performing a quantitative analysis of the impact on the control of the downstream NO₃-N concentration. These strategies would be implemented by a combination of joint operations of the reservoirs with SWF and simulation results with the water quality model.

As mentioned earlier, the methodology presented in this study can be used in further research for the indirect regulation of HABs in rivers by controlling the NO₃-N concentration. Since HABs are produced by various factors such as climate, aquatic environments, etc., many researchers have tried to find the major drivers to predict HABs [25]. Several previous studies suggested that NO₃-N is one of the key factors underlying HABs [12–14]. Accurate prediction of HABs is not easy because HABs can be produced or faded not only by chemical factors but also by biological processes [19,59,70]. However, for cases when NO₃-N is determined to be a critical factor, appropriate countermeasures against HABs in a river can be introduced by predicting and controlling the NO₃-N concentration, which is relatively easier to simulate than HABs.

However, some studies have surprisingly shown that a low concentration of NO₃-N promotes HABs, although the effect could depend on the species of algae [12,71–73]. If these findings are linked with this study, HABs could be controlled by a reduction in the flow rate released from an upstream reservoir as in Scenarios 1–3 or by an increase in the NO₃-N concentration of the released water as in Scenarios 51 and 52 (highly unusual scenarios and hardly possible in practice). Nevertheless, since the implementation of this strategy may lead to an increase in the downstream NO₃-N concentration, an optimization process is necessary by considering an acceptable standard in the NO₃-N concentration required for drinking water sourced from the river.

All the processes for water quality modelling, such as monitoring, analyzing, predicting, and controlling water quality parameters, are closely related to human health and the stability of aquatic ecosystems [74,75]. This study, however, focused on the modelling process for one water quality parameter (NO₃-N). Further studies should be oriented toward sustainable development in terms of public health and ecological diversity and away from simply focusing on the water quality model. For instance, a water quality model would forecast NO₃-N concentrations in a river. The simulation result could be used for judging whether the concentrations would exceed an acceptable level regarding public health. If exceeding the acceptable level, a decision should be made in advance to reduce the NO₃-N concentrations in the river. A series of these processes would support the sustainable development of human life and aquatic ecosystems.

Moreover, we need to mention the hindrances to this study to be considered in further research. In this study, we tried to clearly understand NO₃-N dynamics depending on the changes in water quantity and quality at the upstream boundary. However, since there

were limitations on available data, we needed to make some assumptions. For example, the concentrations of NH₄-N and NO₂-N required in HEC-RAS were replaced with the measured concentration of NH₃-N and zero, respectively [62–67]. Despite these reasonable assumptions based on observable facts, the developed model may still have uncertainty. Furthermore, the HEC-RAS model has not been widely used as a water quality model, although it has been frequently used for flow analysis. This would mean that it should be further validated as a water quality model. In this study, we attempted to develop the HEC-RAS model to simulate the NO_3 -N dynamics in the Nakdong River, but its suitability for simulating other water quality parameters should be further demonstrated. Additionally, we constructed a one-dimensional model with HEC-RAS, but a multi-dimensional model would be necessary for detailed analysis of critical locations (e.g., weirs close to water supply intakes, such as the Chilgok Weir in this study). This is because the fate and transport of NO₃-N may tend to vary in a transverse or vertical direction and not only in a longitudinal direction as modelled in this study. Further studies could be conducted with consideration for adequate substitutes for the data that were not measured, the limitations of the HEC-RAS model as a water quality model, and the application of a multi-dimensional model.

5. Conclusions

We developed a one-dimensional process-based model to simulate the fate and transport of NO₃-N using HEC-RAS for the upper reach of the Nakdong River in South Korea. Variations in the downstream NO₃-N concentration were simulated by the developed model according to changes in water quantity and quality at the upstream boundary. For the monitoring station located near the Chilgok Weir, these simulation results were analyzed in comparison with the modelling result that was obtained using the observational data as boundary conditions without the change in water quantity and quality.

The main finding in connection with the control of water quality is that the change in the downstream NO₃-N concentration was mostly achieved by direct control of the NO₃-N concentration at the upstream boundary. In terms of the control on water quantity, we could create a more significant impact on the change in the downstream NO₃-N concentration by increasing the flow rate at the upstream boundary. However, the reducing effect on the NO₃-N concentration varied depending on how long the flow rate increased and the current status of the downstream NO₃-N concentration. Therefore, strategic decisions on WQM should be made after predicting what effect will be achieved using a water quality model.

Based on the guidelines for the design of strategies for controlling the downstream NO₃-N concentration, we learned that the unilateral decision between water quantity and quality at the upstream boundary would not be best for the improvement in downstream water quality. In this respect, further research can be conducted on the optimal operation of reservoirs in consideration of both water quantity and quality. This optimization process can be accelerated together with a surrogate model for water quality based on a broad spectrum of scenarios.

Author Contributions: Conceptualization, D.P.S., A.J. and J.K.; methodology, D.P.S., A.J. and J.K.; software, J.K.; validation, A.J. and J.K.; formal analysis, J.K.; investigation, A.J. and J.K.; data curation, J.K.; writing—original draft preparation, J.K.; writing—review and editing, D.P.S., P.L.M.G. and A.J.; visualization, J.K.; supervision, D.P.S., P.L.M.G. and A.J. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding. The APC was funded by Delft University of Technology.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The raw data are publicly available at http://www.wamis.go.kr for hydraulic data (accessed on 14 March 2022), https://water.nier.go.kr for water quality data (accessed on 30 March 2022), and https://data.kma.go.kr for meteorological data (accessed on 18 April 2022).

Acknowledgments: We thank K-water (Korea Water Resources Corporation) for financially supporting the first author.

Conflicts of Interest: The authors declare no conflict of interest.

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