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A simulation-optimization approach for assessing optimal wastewater load allocation schemes in the Three Gorges Reservoir, China

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Abstract

Background: The Three Gorges Reservoir (TGR) has been facing deteriorated water quality issues since the construction of the Three Gorges Dam (TGD) in 1994. However, no previous studies have used a simulation-optimization assessment framework to examine the waste-load allocation patterns in the TGR area for alleviating its water pollution problem. In this study, a simulation-optimization modeling approach was developed for addressing this issue, through combining an environmental fluid dynamic code (EFDC)-based water quality simulation model and a waste-load allocation optimization model into a general framework.

Results: The approach was applied to a TGR section (Changshou-Fuling section) for identifying the optimal waste-load allocation schemes among its 11 wastewater discharge outlets. Firstly, the EFDC model was run to simulate the water quality response in the receiving water body under a single discharge load scenario, and the simulated COD and NH_4^+-N concentrations were used to calculate the pollution mixing zone (PMZ), the pollution mixing zone per unit load (PMZPL), and sensitivity index (SI) pertaining to that outlet. These values were then used in the formulation of the waste-load allocation optimization model, with its objective being to maximize the environmental performance under constraints that existing waste discharge loads in terms of total wastewater amount, total pollutant mass, and existing PMZ size can't be exceeded.

Conclusions: Modeling results give an optimal waste-load allocation ratio for each discharge outlet within the study section, and its implications to the reservoir water quality management were analyzed. It is anticipated that the develop approach can be extended to the entire TGR area for better water quality management studies and practices.

Keywords: Environmental fluid dynamic code (EFDC); Water quality simulation; Waste-load allocation optimization; Simulation-optimization approach; Three Gorges Reservoir

Background

The Three Gorges Dam (TGD) spans the Yangtze River by the town of Sandouping, located in the Yiling District of Yichang City, in Hubei province, China. It is a hydroelectric dam and the world's largest power station in terms of installed capacity (21,000 MW). The TGD construction started in 1994 and the dam body was completed in 2006. Since then, the water level behind the dam has gradually increased and reached its designed maximum level of 175 m in October 2010. When the water level is at its maximum, the upstream of the Three Gorges Reservoir (TGR) along the Yangtze River is about 660 km in length and has an average of 1.12 km in width. The TGR contains 39.3 billion m^3 of water with a total surface area of 1,045 km^2, and the reservoir watershed has a total area of 58,000 km^2 (CWRC Changjiang Water Resource Commission 1997). The TGR is situated within an attitude of E106°–115° 50′ and N29°16′–31°25′, as shown in Figure 1. It encompasses 26 towns or counties under the jurisdiction of Metro Chongqing Municipality and Hubei Province, with a total population of 20.1 million.

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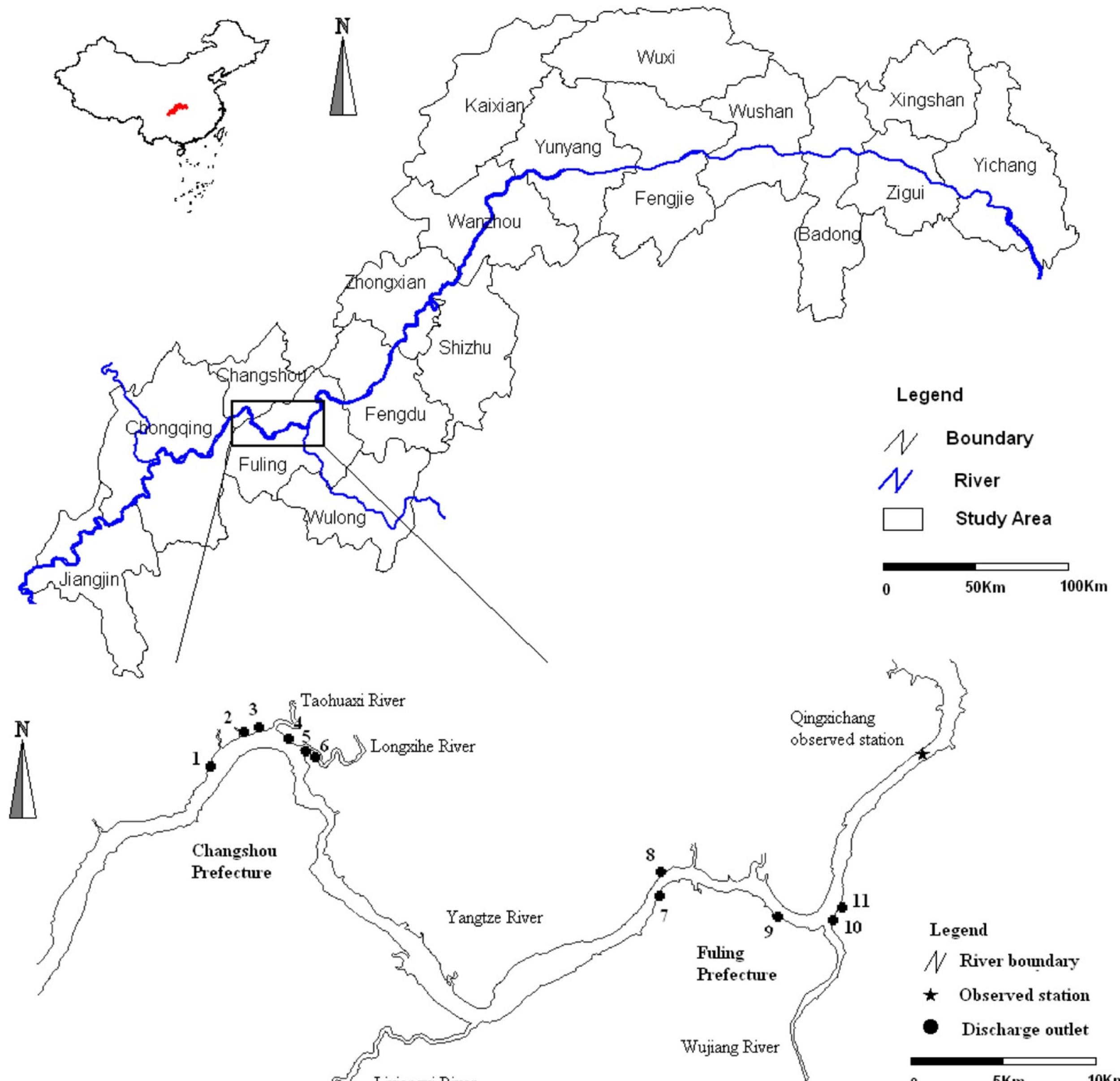

Figure 1 The Three Gorges Reservoir area (top graph), the study reservoir section (bottom graph), and location of 11 industrial wastewater discharge outlets along the study reservoir section (bottom graph).

As the consequences of fast population growth and rapid economic development in the past two decades in the TGR watershed, more and more industrial wastewater and domestic sewage are generated and discharged into the TGR, leading to the deterioration of water quality in the reservoir. Meanwhile, the construction and completion of TGD has resulted in significant changes of hydraulics of water flow in the reservoir, which further affects the transport and fate of various contaminants discharged into the reservoir water body. For example, the advective and diffusive transport of the chemicals in the reservoir water body has been significantly affected due to the slowdown of water flow. As a result, local authorities have been undertaking enhanced stresses in order to effectively respond to these concerns. In general, one reliable path is through designing effective environmental management schemes for dealing with this dilemma, and this requires a sound understanding of the significant contributors to the reservoir water pollution problem, and of the way the reservoir system will react to particular schemes or policies. It becomes obviously desired to study sound allocation schemes for better water quality management in the region.

Generally, the waste-load allocation problems are to determine the allowed discharge levels or required removal levels from a number of point pollution sources in a basin to achieve satisfactory (or aspired) water-quality responses in the receiving water body. Previously, the optimal allocation of waste loads has been typically solved by developing various forms of optimization models Mujumdar and Vemula 2004; Yang et al. 2011; Qin and Xu 2011). The decision variables in the optimization models are the discharge (or removal) levels of wastewater or pollutants at each of the point pollution sources. The objective function is often to maximize economic return or to minimize the treatment cost while the constraints are to ensure that the resulting water-quality responses in the receiving water body are satisfactory. Since the resulting water-quality responses in the receiving water body can only be quantified by water quality simulation models, the waste-load allocation problems are essentially required to conduct a simulation-optimization assessment of levels of waste load reductions and allocations from various sources while ensuring the water quality standards being satisfied. Examples of such studies include a waste load allocation model developed by Cho et al. (2003) for the heavily polluted Gyungan River in South Korea, where a modified QUAL2E model was used for the water quality simulation, and a simulation–optimization analysis of waste load allocation for a river water quality management by Mujumdar and Vemula (2004). In the TGR area, previously, many optimization modeling studies have been conducted but mainly focused on Yangtze River flood control (Cai et al. 2010), hydropower generation (Guo et al. 2011), Yangtze River watershed navigation (Wang and Ruan 2011), and regional water resources allocation and supply (Sun and Lv 2010).

The resulting water-quality response in the receiving water body depends on the total waste load discharged and allocation pattern among different sources, as well as the various hydraulic conditions within the water body. Surface water quality models have been deemed as sound engineering tools for rationalizing water quality management (Chapra 2003; Igbinosa and Okoh 2009; Chen et al. 2010). Various surface water quality modeling studies and software have been carried out and developed for supporting the management of surface water systems, and examples include the river and stream water quality model (QUAL2K) (Chapra et al. 2007), water quality analysis simulation program (WASP) (Wool et al. 2001), environmental fluid dynamics code (EFDC) (Tetra Tech I 2007) and MIKE11 (DHI 2003). Some models can tackle the problems related to chemical and biological processes through deterministic partial differential equations (Igwe et al. 2008; Shah et al. 2009). All the models include two essential components for executing two core tasks: (1) a hydrodynamic sub-model to simulate the water flow circulation and behavior, and (2) a mass transport and kinetics sub-model to simulate the fate and movement of pollutants in the target water bodies. For the TGR area, previous water quality modeling studies have been focused on the simulation of 1D and 2D hydraulic flow in the mainstream of Yangtze River (Huang 2006), analysis of the natural assimilative capacity and water environmental capacity, definition and calculation of pollution mixing zones (Jiang et al. 2005), and some others (Zhao et al. 2011).

Literature survey show that, although the water pollution issue in the TGR has become more and more serious since the construction of the TGD, no previous studies have used a simulation-optimization assessment framework to examine the waste-load allocation patterns in the TGR area for alleviating TGR's water pollution problem. The objective of the present work is thus to combine a water quality simulation model and waste-load allocation model into a general methodology framework, and aims to address the water pollution issue in the TGR area. In this study, the Changshou-Fuling section is a typical mainstream section along the Yangtze River and was selected as the target study section for implementing the modeling runs and identifying the optimal waste-load allocation schemes. The EFDC model was used as the surface water quality model to simulate the flow hydrodynamics and chemical transport. It helps rank and screen the major waste discharge outlets within the study reservoir section. The pollutant mixing zone (PMZ) formed by one single outlet for different pollutants was calculated to establish the linkage between the pollution plume size with the strength of each discharge outlet, and a sensitivity index can then be calculated based on the calculated PMZ. The spatial and temporal distribution of PMZ was calculated by the EFDC model. The waste-load allocation patterns were obtained through optimizing the sensitivity index of each waste discharge outlet. According to the modeling results, the schemes for optimal waste-load allocations among 11 different discharge outlets were analyzed. The implications to formulate the strategies for improving the water quality for the entire region were also discussed. It is anticipated that the methodology developed in this study can be extended to other TGR areas for better water quality management studies and practices.

The Changshou-Fuling reservoir section

The Changshou-Fuling section of the TGR was selected as the study area, as shown in Figure 1. It is subject to a tropical monsoon climate of Northern Asia and has an annual mean temperature of 18°C, an average precipitation of 1170 mm per year, and an average evaporation of 1300 mm per year, and an average wind speed of 1.4 m/s (Zhao et al. 2011). This reservoir section has an annual mean flow velocity of 0.8 m/s, a mean flow rate of 12,000 m^3/s, and a mean water depth of 50 m (MWRC Ministry Of Water Resources of China 2008). Changshou and Fuling Districts are two major industrial bases of ChongQing Municipality. They have a total of 11 industrial wastewater discharge outlets located along the study section, discharging a large amount of untreated industrial wastewater into the TGR. Among them, 6 discharge outlets are located in Changshou District and the other 5 are located in Fuling District (as indicated in Figure 1, bottom graph, and Figure 2). The study section is approximately 90 km long, with 18 km located in Changshou District in the upper reach and 72 km in Fuling District in the lower reach. The Wujiang River flows into this section right before the discharge outlet #10 and is the second largest inflow tributary of the TGR. Figure 3 gives a digital elevation map of the study reservoir section. With the rapid population growth and fast economic growth in the past two decades, the overall water quality of in the

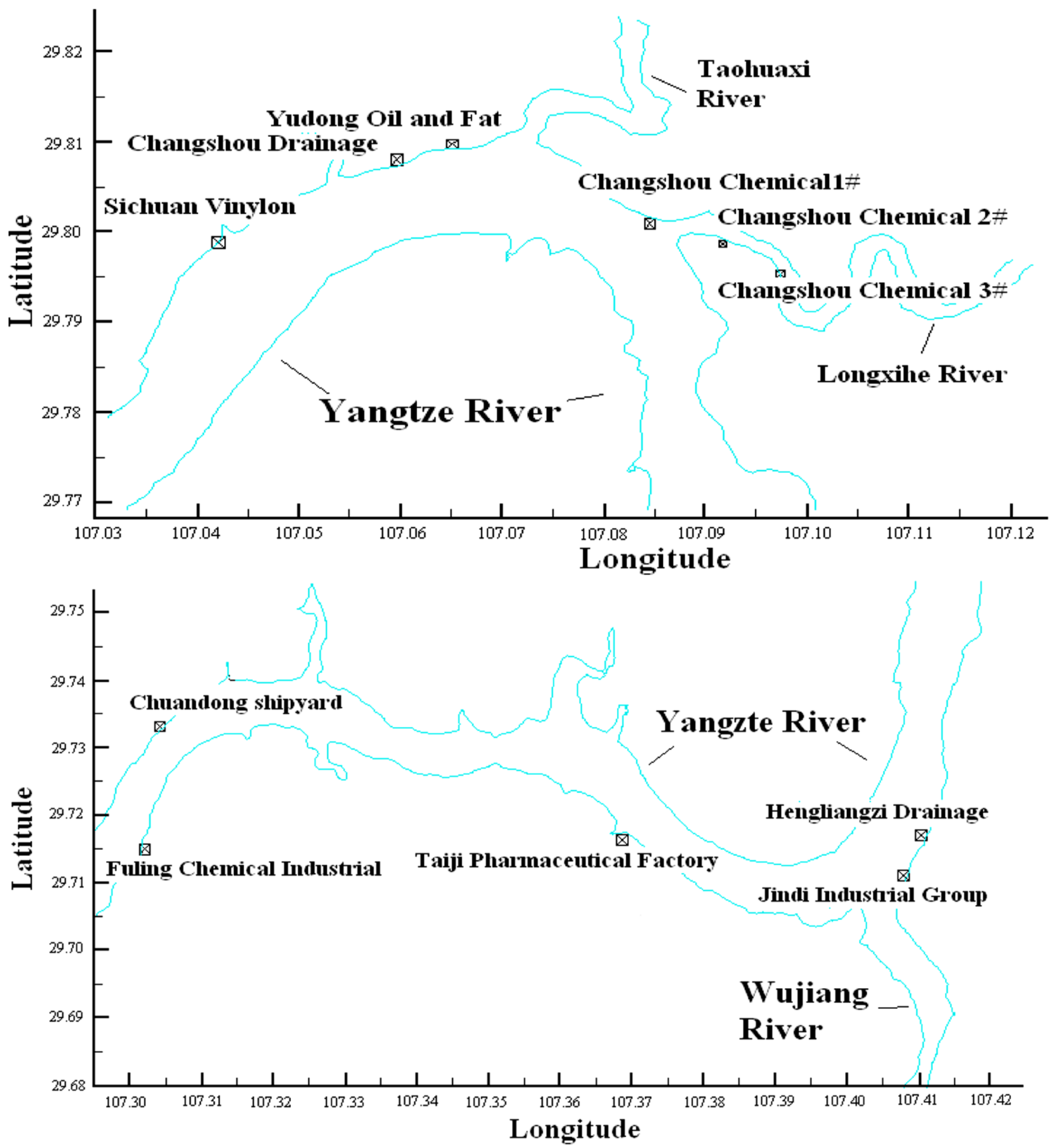

Figure 2 Locations of 11 discharge outlets in the study reservoir section (top: Changshou section; bottom: Fuling section).

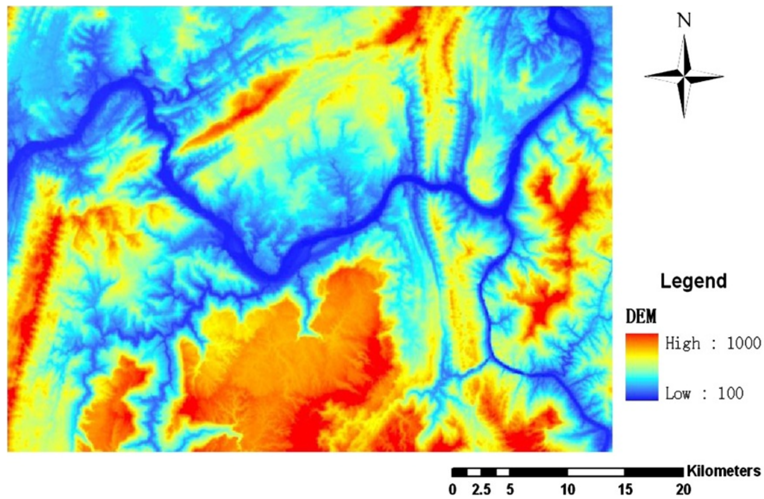

Figure 3 Digital elevation map of the study reservoir section.

Changshou-Fuling section has been gradually deteriorated and has been in very poor conditions (Yibing et al. 2007). Furthermore, the construction and completion of the TGD have made the situation even worse.

In this study, a topographic map with a resolution of 1:25,000 was used to delineate the river channel characteristics, and the water depth along the study section was sourced from the Department of Hydrology, Changjiang Water Resources Commission (Changjiang WRC). Hydrological data were obtained from the Bureau of Hydrology, the Ministry of Water Resources of China (MWRC). Water quality data include the concentrations of DO, COD, NH_4^+-N, observed at the Qingxichang monitoring station in 2008, and were provided by the ChongQing Environmental Science Research Institute. Meteorological data were downloaded from the website of the China Meteorological Data Sharing Service System. Industrial and municipal point pollution source data for 2008 for Changshou and Fuling Districts were provided by the Changjiang Water Resources Protection Institute. Data of nutrients (N, P) from non-point sources within the study section were provided by Chongqing Environmental Science Research Institute. The Level-II water quality standard specified in the National Environmental Quality Standards for Surface Water (GB3838-2002) was applied, and the standards for NH_4^+-N and COD are 0.5 mg/L and 15 mg/L, respectively. The discharge load from each discharge outlet in the year of 2008 is given in Table 1.

Methods

The simulation-optimization assessment approach

Definitions of pollutant mixing zone (PMZ) and sensitivity index (SI)

Before we discuss how the surface water quality simulation model and waste-load allocation model was combined into a general assessment framework, a few concepts need to be defined. A primary concept is the pollution (or pollutant) mixing zone (PMZ), and it was defined as the area of a contamination plume caused by the wastewater discharge where the water quality within the zone exceeds the Level-II national surface water quality standards. The area of the PMZ for each discharge outlet is affected by their respective factors, mainly including the discharge load from the outlet, hydro-dynamic flow feature around the outlet, natural assimilative capacity of local water body, and background concentrations of the pollutants of interest. It was calculated by the EFDC model. The pollutant mixing zone per unit load (PMZPL) can then be defined and calculated by:

$$PMZPL_i = \frac{PMZ_i}{DL_i} \tag{1}$$

where PMZ_i is the surface area of the pollutant mixing zone formed by the ith discharge outlet (in m^2); DL_i

Table 1 Discharge load from 11 discharge outlets in 2008

Number	Discharge outlet	District	Discharge load (kg/d)	
			COD	NH_4^+-N
1	Sichuan Vinylon	Changshou	6959	316
2	Changshou Drainage	Changshou	1200	100
3	Yudong Oil and Fat	Changshou	1225	82
4	Changshou Chemical #1	Changshou	1927	551
5	Changshou Chemical #2	Changshou	628	338
6	Changshou Chemical #3	Changshou	1372	677
7	Fuling Chemical Plant	Fuling	7778	1399
8	Chuandong shipyard	Fuling	295	38
9	Taiji Pharmaceutical Factory	Fuling	562	15
10	Jindi Industrial Group	Fuling	522	68
11	Hengliangzi Drainage	Fuling	2055	205

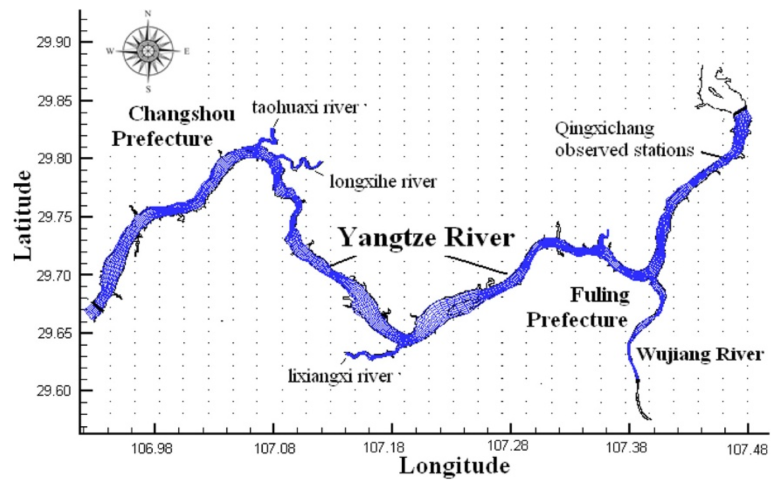

Figure 4 The computation grid designed for the Changshou-Fuling reservoir section.

refers to the discharge load from the *i*th discharge outlet (in kg/day).

In this study, the monthly and annually average values of PMZ and PMZPL for each individual discharge outlet were calculated by the EFDC-based water quality simulation model. In a specific PMZ calculation, only the discharge load from the outlet of interest was considered and used in the EFDC simulation, while the discharge loads from all other outlets were assumed to be zero. As a result, the calculated PMZ and MPZPL only reflect the pollution contribution from each individual outlet. A sensitivity index can then be defined to indicate how sensitive or important each individual discharge outlet could be among all the outlets in terms of its impact on water pollution. The formula to calculate the sensitivity index for each outlet is given below:

$$SI_i = \frac{PMZR_i}{DLR_i} \tag{2}$$

Where SI_i is the sensitivity index for the *i*th discharge outlet (dimensionless); $PMZR_i$ is the ratio or share of the PMZ formed by the *i*th outlet to the total PMZ area formed all the outlets (dimensionless); and DLR_i represents the ratio or share of the discharge load from the *i*th outlet to the total discharge load from all the outlets (dimensionless). It is indicated that a higher SI value means a bigger PMZ area influenced by a specific outlet and a stronger pollution impact from the same outlet. $PMZR_i$ and DLR_i can be calculated by the following two formulas:

$$PMZR_i = \frac{PMZ_i}{\sum_{i=1}^{n} PMZ_i} \tag{3}$$

$$DLR_i = \frac{DL_i}{\sum_{i=1}^{n} DL_i} \tag{4}$$

In Equations (3) and (4), the subscript *i* indicates the number of discharge outlet along the study reservoir section. In this study, there are a total of 11 outlets ($n = 11$).

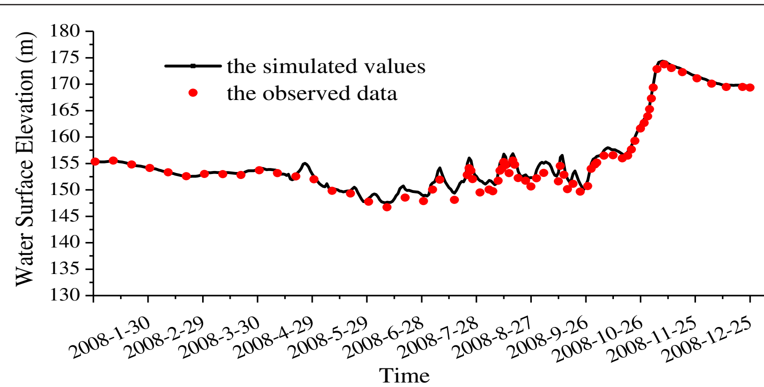

Figure 5 Comparison of simulated and observed water levels at Qingxichang monitoring station in 2008.

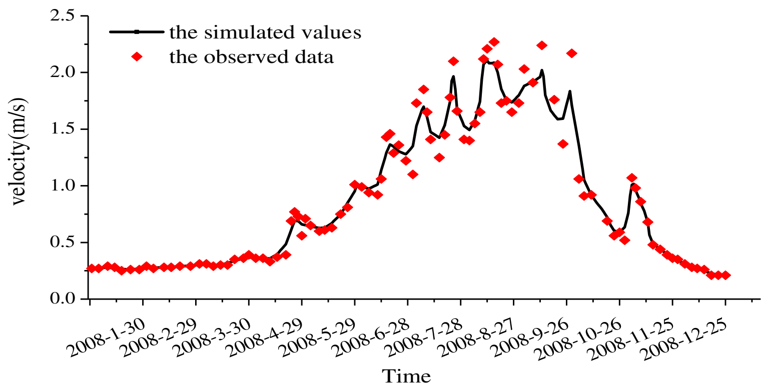

Figure 6 Comparison of simulated and observed flow velocity at Qingxichang monitoring station in 2008.

Simulation-optimization assessment framework

In this study, a hydro-dynamic water quality simulation model was developed using the environmental fluid dynamics code (EFDC) (Tetra Tech I 2007). The EFDC-based simulation model was used to calculate the monthly and annually average value of PMZ formed by each individual discharge outlet. The discharge load from one individual outlet was used as the single load input in each run of the EFDC simulation. Also, a linear optimization model was formulated to seek the optimal waste-load allocation schemes among different discharge outlets within the study section. In this study, the water quality simulation and waste-load allocation model were then combined into a general assessment framework. The assessment process was carried out in a sequential manner. It starts with running the EFDC simulation model to provide the values of parameters used in the optimization model, and then the optimization model was run to search for the best waste-load allocation schemes. The details of the modeling and assessment processes are proved in the following context.

EFDC-based water quality simulation modeling

Model description

The EFDC is a public domain, open source, surface water modeling system, and includes hydrodynamic, sediment and contaminant, and water quality modules which are fully integrated in a single source code implementation. EFDC has been applied to over 100 water bodies including rivers, lakes, reservoirs, wetlands, estuaries, and coastal ocean regions in support of environmental management and regulatory requirements. The EFDC was originally developed at the Virginia Institute of Marine Science (VIMS) and the School of Marine Science of The College of William and Mary, by Dr. John M. Hamrick in 1988 (Tetra Tech I 2007). The hydrodynamics of the EFDC is based on the Princeton Ocean Model; the physics of the two models are the same (Blumberg and Mellor 1987).

For simulating the water quality, the EFDC solves the hydrodynamics and drives the transport of chemicals by using the hydrodynamic results. The water quality module in the EFDC solves the phytoplankton kinetics, which includes nutrient uptake, growth, respiration, discretion,

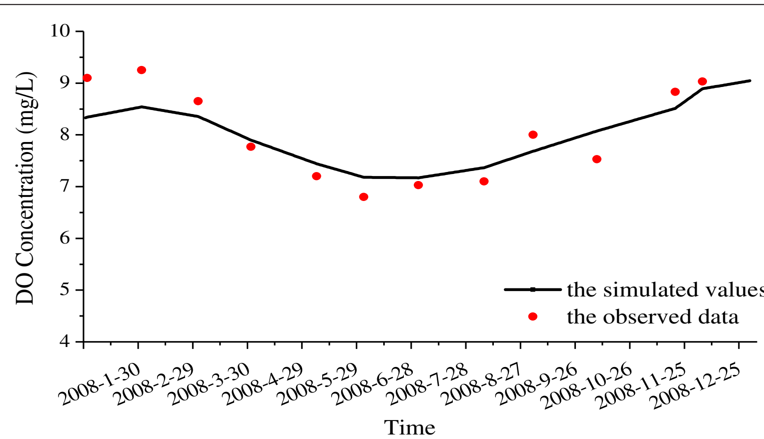

Figure 7 Comparison of simulated and observed DO concentration at Qingxichang monitoring station in 2008.

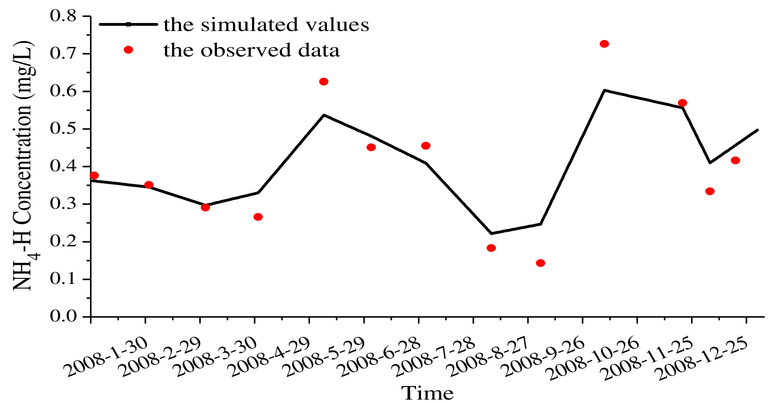

Figure 8 Comparison of simulated and observed NH_4^+-N concentration at Qingxichang monitoring station in 2008.

settling processes and nutrient transformations. The EFDC water quality module is based on CE-QUAL-ICM and can simulate up to 22 state variables (Hamrick 1996). The governing mass-balance equation for each of the water quality state variables is expressed as in the Equation (5).

$$\frac{\partial(m_x m_y HC)}{\partial t}+\frac{\partial(m_y HuC)}{\partial x}+\frac{\partial(m_x HvC)}{\partial x}+\frac{\partial(m_x m_y wC)}{\partial x} = \frac{\partial}{\partial x}\left(\frac{m_y HA_x}{m_x}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{m_x HA_y}{m_y}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{m_x m_y A_z}{H}\frac{\partial C}{\partial z}\right)+S_c \quad (5)$$

Where, C denotes the concentration of a water quality state variable; u, v, and w refer to the velocity components in x-, y-, and z-directions in generalized curvilinear and sigma coordinate systems; A_x, A_y, A_z are the turbulent diffusivities in the x-, y-, and z-directions, respectively; H is the water column depth; m_x, m_y are the horizontal curvilinear coordinate scale factors; S_c represents internal and external sources and sinks per unit volume, which are either generated and/or consumed by kinetic processes. The kinetic formulations of water quality component in the EFDC are primarily from CE-QUAL (Hamrick 1996).

Model setup

A horizontal computation grid was designed for the study reservoir section and for running the EFDC model, as shown in Figure 4. In this study, the orthogonal curvilinear grids were used for setting up the EFDC model to fit the natural flow boundary. The model maps the orthogonal curvilinear grid with the software Delft3D (Zuo 2007). The designed grids consist of 4373 cells in the horizontal direction, with grid size ranging from 10 m to 300 m. A vertical sigma coordinate was evenly distributed by 5 layers for better simulating the bottom topography (Xie et al. 2010). Model simulation time step was set to 5 s. For the initial conditions, the water surface elevation for each active cell was set to 155 m and the water quality variables for each active cell were set same to the initial data (Wu and Xu 2011; Zhao et al. 2011; Parka et al. 2005; Li et al. 2011).

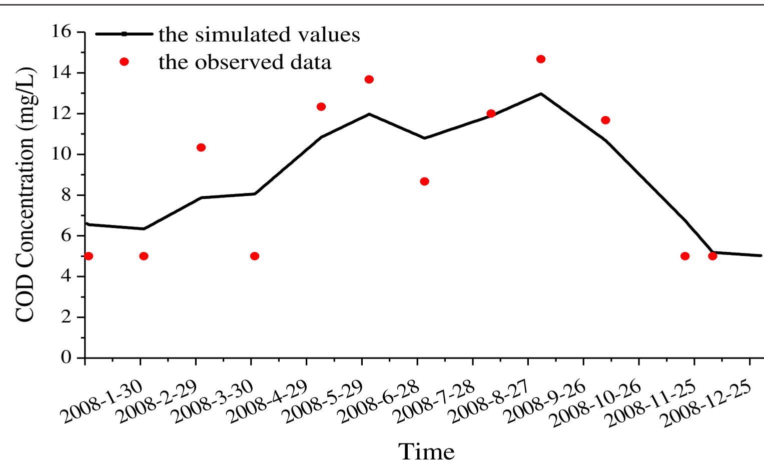

Figure 9 Comparison of simulated and observed COD concentration at Qingxichang monitoring station in 2008.

Table 2 Error analysis between simulated and observed verification parameters

Variable	Mean error	Absolute mean error	Absolute relative mean error
Water surface level (m)	0.081	1.004	0.65%
Velocity (m/s)	0.048	0.058	5.53%
DO (mg/L)	0.073	0.353	4.34%
NH_4^+-N (mg/L)	0.008	0.051	16.51%
COD (mg/L)	0.233	1.537	20.94%

Model verification

To verify the EFDC model, the simulated results were compared with the field water quality data observed in the year of 2008 at the Qingxichang Monitoring Station. The parameters used for model verification include two hydrodynamic variables (i.e., water level and flow velocity) and three water quality variables (i.e., concentrations of DO, NH_4^+-N and COD), all of which are on a daily average basis. The field data were collected on a monthly basis and the daily average was recorded for each monitored parameter.

Figures 5, 6, 7, 8 and 9 present the model verification results in terms of water levels, flow velocity, DO concentration, NH_4^+-N concentration and COD concentration, respectively. The mean error, absolute mean error and absolute relative mean error for each comparison are also calculated and given in Table 2. The model verification results indicate that the simulated and observed hydrodynamic variables are in excellent agreements. For three water quality variables as indicated in Figures 7, 8 and 9 and Table 2, bigger discrepancies were observed, particularly for NH_4^+-N concentration and COD concentration. However, considering the inherent uncertainties and complexities involved in water quality simulation process, this level of discrepancy are still acceptable and are regarded within the satisfactory range. According to the model verification results, it is believed that the developed EFDC-based model can be applied to the hydrodynamic and water quality simulation for the study reservoir section.

Waste-load allocation optimization modeling

In order to achieve a better environmental performance through optimal waste-load allocation among different outlets, the natural assimilative capacities of the receiving water body near each outlet should be taken into consideration. For example, the field tests show that, the receiving water bodies near the discharge outlets at Changshou Chemical Plant #1, Hengliangzi Drainage, and Fuling Chemical plant, has high capacities in diluting COD by physical advection–diffusion mechanisms and chemical and biological degradation; while the receiving water bodies near the other 8 discharge outlets have higher capacities in diluting the ammonia-nitrogen (NH_4^+-N). For formulating the optimization model, a concept of environmental performance index (EPI) was defined to reflect combined effects of the waste load level from each outlet and the assimilative capacity of the receiving water body near the outlet. Its magnitude represents the relative importance of each outlet in improving water quality with its discharge load being optimally allocated.

The values of the EPI were determined by the AHP (analytic hierarchy process) approach. This approach decomposes the original problem into a hierarchy of more easily comprehended sub-problems, each of which can be analyzed independently. An AHP hierarchy generally consists of an overall goal, a group of options or alternatives for reaching the goal, and a group of factors or criteria that relate the alternatives to the goal. In this study, the overall goal is the overall water quality improvement and performance in the reservoir; the group of alternatives refers to the 11 discharge outlets and their calculated SI

Table 3 The simulated PMZ values and the calculated values of DLR, PMZR and SI for each discharge outlet

Discharge outlet	COD				NH_4–H			
	DLR	PMZ (m^2)	PMZR	SI	DLR	PMZ (m^2)	PMZR	SI
Sichuan Vinylon	28.38%	70331.72	32.29%	**1.14**	8.34%	8196.08	9.02%	**1.08**
Changshou Chemical #1	7.86%	15560.12	7.14%	**0.91**	14.54%	11215.92	12.34%	**0.85**
Changshou Chemical #2	2.56%	8882.03	4.08%	**1.59**	8.92%	12465.81	13.72%	**1.54**
Changshou Chemical #3	5.59%	17469.15	8.02%	**1.43**	17.87%	26242.91	28.88%	**1.62**
Changshou Drainage	4.89%	13042.31	5.99%	**1.22**	2.64%	2468.27	2.72%	**1.03**
Yudong Oil and Fat	5.00%	13513.16	6.20%	**1.24**	2.16%	1942.11	2.14%	**0.99**
Hengliangzi Drainage	8.38%	19770.31	9.08%	**1.08**	5.41%	5062.12	5.57%	**1.03**
Fuling Chemical Plant	31.72%	43934.76	20.17%	**0.64**	36.92%	20195.29	22.23%	**0.60**
Taiji Pharmaceutical Factory	2.29%	6234.39	2.86%	**1.25**	0.40%	398.97	0.44%	**1.11**
Jindi Industrial Group	2.13%	5812.61	2.67%	**1.25**	1.79%	1946.98	2.14%	**1.19**
Chuandong shipyard	1.20%	3269.58	1.50%	**1.25**	1.00%	728.92	0.80%	**0.80**

Table 4 The derived EPI values for each outlet by the APH approach

Discharge outlet	EPI values
Sichuan Vinylon	0.0843
Changshou Chemical #1	0.1068
Changshou Chemical #2	0.0593
Changshou Chemical #3	0.0581
Changshou Drainage	0.0868
Yudong Oil and Fat	0.0895
Hengliangzi Drainage	0.0885
Fuling Chemical Plant	0.1515
Taiji Pharmaceutical Factory	0.0811
Jindi Industrial Group	0.0766
Chuandong shipyard	0.1075

values (as presented in Table 3). These alternatives are related to the overall goal through two water pollutants, i.e., NH_4^+-N and COD. Once the hierarchy was built, various alternatives were systematically evaluated by comparing them to one another two at a time, with respect to their impact on a factor above them in the hierarchy. In making the comparisons, both concrete data about the alternative and any experience about the alternative' relative importance could be used. The AHP converts these evaluations and comparisons to numerical values that can be processed and compared over the entire range of the problem. In this study, the derived EPI values are presented in Table 4, and they represent a comprehensive and rational ranking for the discharge outlets in terms of their important and weight in contributing to water quality improvement in the study section.

With the EPI being defined, a linear programing model was then formulated to search for the optimal waste-load allocation schemes. The decision variable is the ratio or percentage of wastewater discharge amount from one specific outlet over the total wastewater amount discharged from all the outlets. For this problem, our goal aims to achieve a best water quality improvement result, and thus, the objective function of the linear model is to maximize the overall environmental performance achieved by optimally allocating the wastewater discharge among all the outlets. The overall environmental performance is mathematically represented by the sum of the product of decision variable and the corresponding EPI for all the outlets. The optimal solutions are searched under a number of constraints that the existing pollution situations could be exceeded. The existing pollution situations were expressed in terms of total wastewater discharge, total pollutants discharge, and existing PMZ plume size. Also, the discharge ratio for each outlet is pre-determined in a certain range. The complete linear waste-load allocation model is presented below:

Objective function:

$$\text{Max } F = \sum_{i=1}^{11} \alpha_i x_i \tag{6a}$$

Subject to:

(1) PMZ constraint for pollutant COD

$$\sum_{i=1}^{11} \left(M\beta_{iCOD}\gamma_{iCOD}\right) x_i \leq S_0\_COD \tag{6b}$$

(2) PMZ constraint for pollutant NH_4^+-N

$$\sum_{i=1}^{11} \left(M\beta_{iNH_4^+-N}\gamma_{iNH_4^+-N}\right) x_i \leq S_0\_NH_4^+-N \tag{6c}$$

(3) Total COD discharge constraint

Table 5 Numeric values of the parameters used in the linear optimization model

Discharge outlet	γ_{iCOD} [m²/(kg/d)]	$\gamma_{iNH_4^+-N}$ [m²/(kg/d)]	β_{iCOD} [kg/m³]	$\beta_{iNH_4^+-N}$ [kg/m³]	Q_COD [kg/d]	$Q\_NH_4^+-N$ [kg/d]	Q_WW [m³/d]
Sichuan Vinylon	10.11	25.94	0.11	0.005	6959	316	63260.27
Changshou Chemical #1	8.07	20.36	0.158	0.045	1927	551	12196.16
Changshou Chemical #2	14.14	36.88	0.158	0.085	628	338	3972.6
Changshou Chemical #3	12.73	38.76	0.158	0.078	1372	677	8680.55
Changshou Drainage	10.87	24.68	0.06	0.005	1200	100	20000
Yudong Oil and Fat	11.03	23.68	0.158	0.085	1225	82	7753.42
Hengliangzi Drainage	9.62	24.69	0.05	0.005	2055	205	41095.89
Fuling Chemical Plant	5.65	14.44	0.8	0.126	7778	1399	652.05
Taiji Pharmaceutical Factory	11.09	26.60	0.215	0.028	562	15	1369.86
Jindi Industrial Group	11.14	28.63	0.354	0.064	522	68	21945.21
Chuandong shipyard	11.08	19.18	0.56	0.015	295	38	1002.74

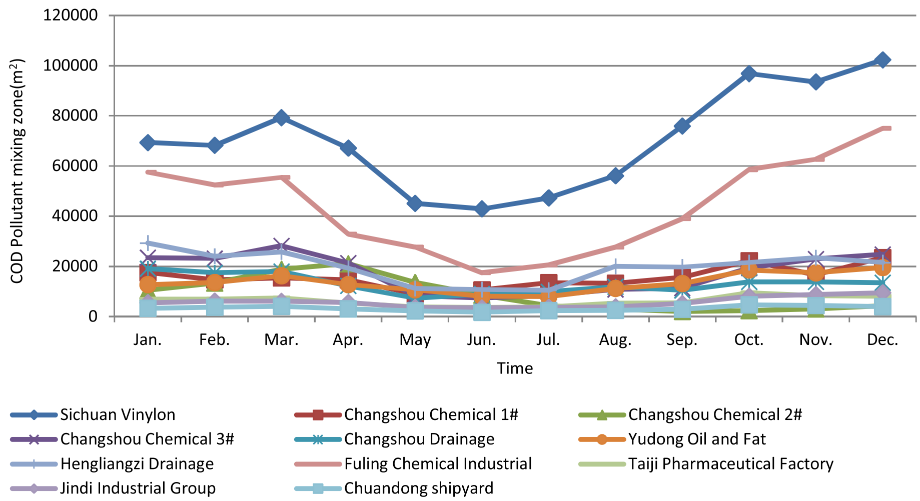

Figure 10 Monthly average size of COD-PMZ formed by each discharge outlet.

$$\sum_{i=1}^{11}(M\beta_{iCOD})x_i \le Q_0\_COD \quad (6d)$$

(4) Total NH_4^+-N discharge constraint

$$\sum_{i=1}^{11}\left(M\beta_{iNH_4^+-N}\right)x_i \le Q_{0N}H_4^+-N \quad (6e)$$

(5) Total wastewater discharge constraint

$$\sum_{i=1}^{11}Mx_i \le Q_0\_WW \quad (6f)$$

(6) Discharge ratio constraints

$$x_i^{\min} \le x_i \le x_i^{\max} \quad (6g)$$

$$\sum_{i=1}^{11}x_i = 1 \quad (6h)$$

(7) Technical constraints

$$x_i \ge 0 \quad (6i)$$

In Model (6), x_i represents the ratio or percentage of wastewater discharge amount over the total amount discharged from all the outlets, and the subscript i represent the 11 discharge outlets along the study section ($i = 1, 2, \ldots, 11$); $x_i^{\max}$ and $x_i^{\min}$ denote the upper and lower limits of x_i, respectively; α_i refers to the EPI for each discharge outlet (dimensionless); M is the total wastewater discharge amount from all the outlets (m^3/d); β_{iCOD} and $\beta_{iNH_4^+-N}$ are the average COD and NH_4^+-N concentrations

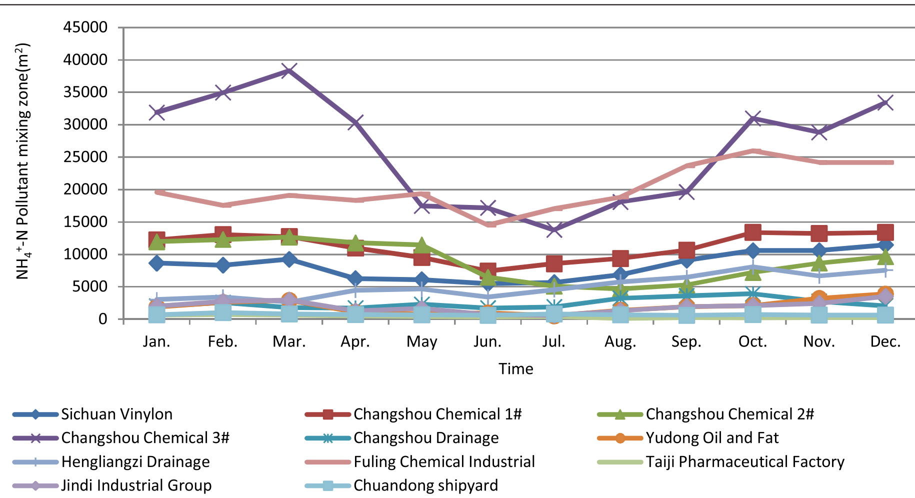

Figure 11 Monthly average size of NH_4^+–H-PMZ formed by each discharge outlet.

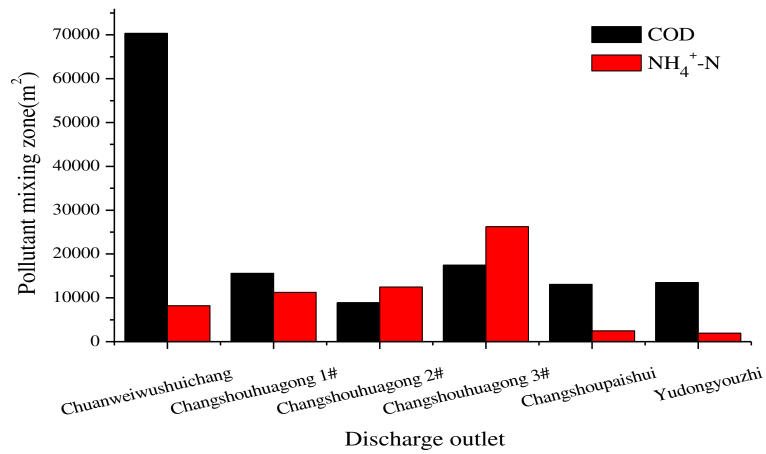

Figure 12 The simulated yearly average size of PMZ formed by 6 outlets in Changshou District.

(in kg/m^3) in the wastewater stream discharged from the ith outlet; γ_{iCOD} and $\gamma_{iNH_4^+-N}$ are the calculated numeric values of the pollutant mixing zone per unit load (in m^2/(kg/d)) for COD and NH_4^+-N for the ith outlet, respectively (i.e., $\gamma_{iCOD} = PMZPL_i$ for COD, and $\gamma_{iNH_4^+-N} = PMZPL_i$ for NH_4^+-N); S_0_COD and $S_{0N}H_4^+-N$ represents the existing plume of the pollutant mixing zone (m^2) in the entire study section for COD and NH_4^+-N, respectively, calculated by the EFDC model; Q_0_COD and $Q_0\_NH_4^+-N$ represents total amount of pollutants COD and NH_4^+-N discharged currently from all the outlets (in kg/d); Q_0_WW is the total wastewater amount discharged currently from all the outlets (in m^3/d). Table 5 gives the numeric values of β_{iCOD}, $\beta_{iNH_4^+-N}$, γ_{iCOD}, and $\gamma_{iNH_4^+-N}$. Table 5 also presents the discharge amount of COD, NH_4^+-N and wastewater from each outlet (i.e., Q_i_COD, $Q_i\_NH_4^+-N$, and Q_i_WW, respectively), and sum of each column equals to their total, Q_0_COD, $Q_0\_NH_4^+-N$, and Q_0_WW, respectively.

Results and discussions

The verified EFDC model was run to calculate the spatial and temporal distributions of monthly average COD and NH_4^+-N concentrations, which were used to calculate the size of PMZ and the value of PMZPL for each outlet. The monthly average size of PMZ formed by each discharge outlet was calculated and presented in Figures 10 and 11, with Figure 10 for COD and Figure 11 for NH_4^+-N. It is apparent that the PMZ size fluctuates from month to month for a specific outlet and is also different from one outlet to another. The calculated PMZ values are the fundamental data for computing other parameters, such as those data presented in Table 5.

The EFDC model was then run to calculate the yearly average size of PMZ for each discharge outlet, and the yearly average PMZPL can then be calculated using Equation (1). They can then be used to calculate DLR and PMZR and SI using Equations (2), (3) and (4). Table 3 gives the simulated PMZ values and the calculated values of DLR, PMZR and SI for each discharge outlet. It is indicated

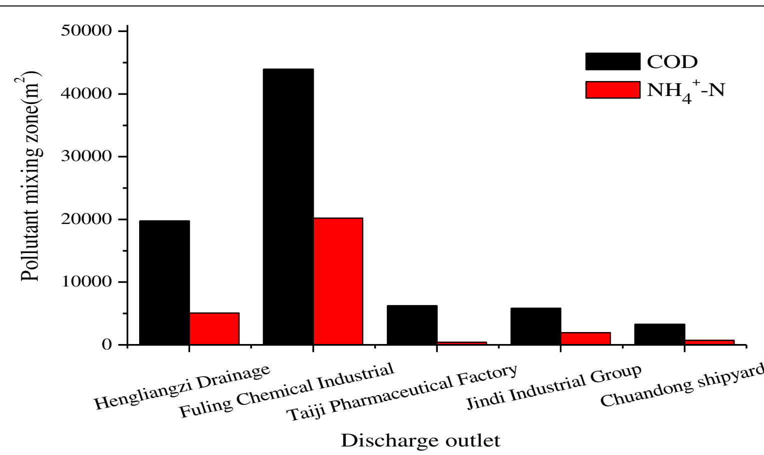

Figure 13 The simulated yearly average size of PMZ formed by 5 outlets in Fuling District.

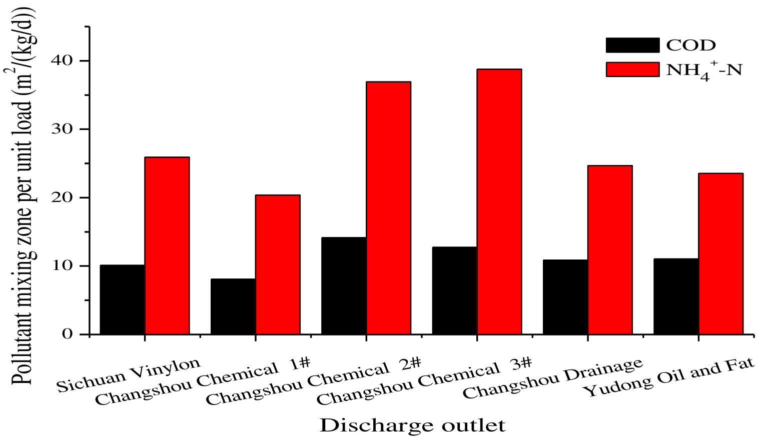

Figure 14 The calculated yearly average of PMZPUL for 6 discharge outlets in Changshou District.

that different discharge outlet has different level of sensitivity index. A higher SI value represents a bigger PMZ area influenced by a specific outlet and a stronger pollution impact from the same outlet. Therefore, the concept of sensitivity index can help rank the significance and influence of a specific discharge outlet on the formation of the pollutant mixing zone in its surrounding water body in comparison to all other outlets. From this sense, a discharge outlet with a high SI has a big potential for improving reservoir water quality if a same level of waste load is cut across the board from all outlets. In other words, this outlet will have a better environmental performance than others if appropriate action is taken for water pollution control purpose.

Based on the data presented in Table 3, the yearly average PMZ size of COD and NH_4^+-N formed by each outlet is plotted as bar graphs in Figures 12 and 13. Figure 12 is the plot for 6 outlets in Changshou District, and Figure 13 is the plot for 5 outlets in Fuling District. In Changshou District, the biggest COD-PMZ was formed near the outlet of Sichuan Vinylon, with an area of 70331.72 m^2, and it account for 51% of the total COD-PMZ formed in the reservoir section in Changshou District. The biggest NH_4^+-N-PMZ was formed near the outlet of Changshou Chemical #3, with an area of 26242.91 m^2, which accounts for 42% of total NH_4^+-N-PMZ formed in Changshou. In Fuling District, the biggest COD-PMZ and NH_4^+-N-PMZ was both formed near the outlet of Fuling Chemical Industrial, with an area of 43934.76 m^2 and 20195.29 m^2, which accounts for 56% and 71% of the total formed in Fuling, respectively.

Similarly, the calculated yearly average of PMZPL for COD and NH_4^+-N is plotted as bar graphs in Figures 14 and 15, respectively. Figure 14 is the plot for 6 outlets located in Changshou District, and Figure 15 is the plot for 5 outlets located in Fuling District. Some interesting observations could be obtained. For example, the biggest yearly average PMZPL for COD appears near the outlet of Changshou Chemical #2 while that for NH_4^+-N is near Changshou Chemical #3. Both discharge outlets are located

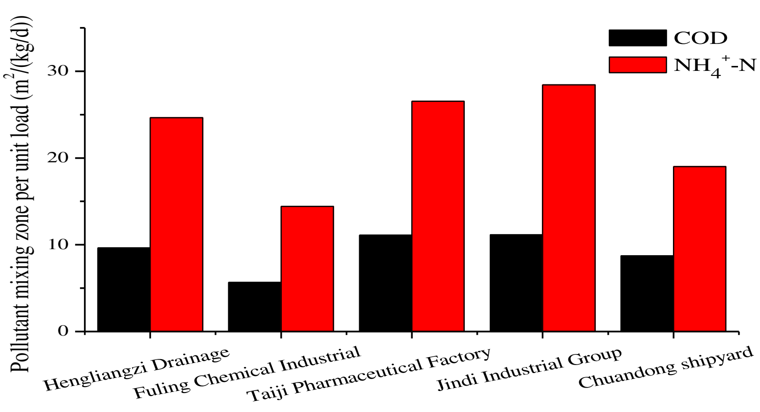

Figure 15 The calculated yearly average of PMZPUL for 5 discharge outlets in Fuling District.

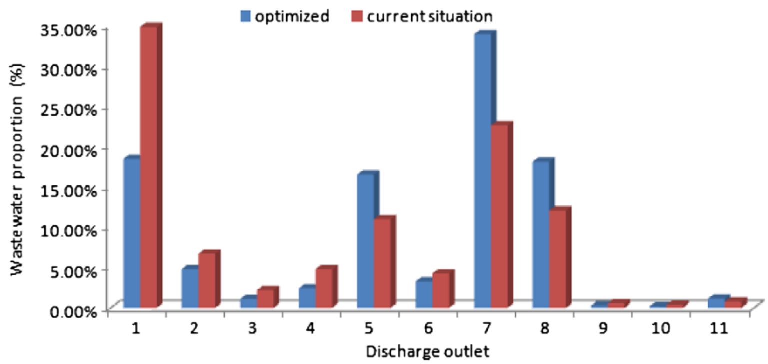

Figure 16 The optimal wastewater allocation result (blue bar graphs) and its comparison with existing discharge load level for each outlet in the study section.

at Longxihe River which is a tributary of the Yangtze River. The return water from the Yangtze River changes the hydraulics of the Longxihe River and might be the main cause of a large PMZ formation. It is also observed from Figure 14 that the PMZPL value of Chemical #2 almost doubles that of Chemical #1. According to the data presented in Tables 1 and 3, the PMZ sizes formed by Changshou Chemical #1 and #2 are very close (11216 m^2 for #1 and 12466 m^2 for #2), however, the NH_4^+-N discharge load from Chemical #1 is 551 kg/d while that from Chemical #2 is only 338 kg/d. There are two possible reasons to explain this: (1) the NH_4^+-N concentration from Chemical #2 is much higher (0.085 kg/m^3) than that from Chemical #1; (2) Chemical #1 is located at the estuary close to mainstream of Yangtze River which make the NH_4^+-N be easily dispersed and diluted.

In this study, the formulated optimization model (6) was solved using Lingo Software. The optimization results give an optimal allocation of wastewater discharge loads among 11 discharge outlets, as presented in Figure 16 and Table 5. A comparison between the existing discharge load level and the optimal load level is also provided. It is indicated that the outlets of Changshou Drainage, Hengliangzi Drainage, and Fuling Chemical Industrial need to increase their discharge load and ratio of the discharge load among the total while the allocation ratios for others need to reduced, for achieving the best environmental performance in terms of reservoir water quality improvement. It is suggested that the management policy and strategy should not only focus on the reduction of industrial wastewater discharge, but also on the increased treatment of domestic wastewater.

Conclusions

In this study, a simulation-optimization assessment framework was developed to help address the water pollution issue in the TGR area, through combining an EFDC-based water quality simulation model and a waste-load allocation optimization model into a general methodology framework. The developed method was applied to the Changshou-Fuling reservoir section for ratifying the approach and identifying the optimal waste-load allocation schemes among its 11 wastewater discharge outlets. After being verified, the EFDC model was used to simulate the flow hydrodynamics and contaminant transport in the study reservoir section. The simulated COD and NH_4^+-N concentrations were used to calculated the size of pollution mixing zone formed at each discharge outlet. The pollution mixing zone per unit load as well as the sensitivity index for each discharge outlet was also calculated to reflect the connections between the pollution plume and the load strength from each outlet. These parameters were used for developing the waste-load allocation optimization model with an objective of maximized environmental performance under constraints that existing waste discharge loads in terms of total wastewater amount, total pollutant weight, and existing PMZ size formed can' t be exceeded. Modeling results give an optimal waste-load allocation ratio for each discharge outlet within the study reservoir section, and its implications to regional water quality management were analyzed. It is anticipated that the methodology developed in this study can be extended to the entire TGR area for better water quality management studies and practices.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

ZW focused on EFDC model setup, formulation, verification, and water quality simulation, and he was also responsible for the waste load allocation optimization model formulation and implementation. SC and LL were the technical advisors for the project, and they were responsible for designing the methodology framework, drafting the manuscript with the help of ZW, participating in modeling studies, and finalizing the project and manuscript. YC focused mainly on the EFDC modeling studies. XG participated in the calculation of pollution mixing zone and sensitivity index. CQ participated in the system analysis for the study reservoir section. RH, JL and JG were on the field trip to the study section for data collection and analysis, and they were also responsible for the modeling result analysis and interpretation. All authors read and approve the final manuscript.

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