A MODEL FOR SIMULATING WATER QUALITY IN A RIVER AND APPLICATION OF GENETIC ALGORITHM IN THE MODEL CALIBRATION

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ABSTRACT: This study focuses on finding the properties of water quality parameters affected by different sources of pollutants along the Tatara River, a small river in Fukuoka city of Japan. Results getting from data analysis pointed out interesting and noticeable properties of water quality in the Tatara River, which is significantly affected by various point sources. The results also indicated the changing tendencies of water temperature and dissolved oxygen in the Tatara River in response to different meteorological conditions over a daily cycle. On the other hand, we developed and applied a numerical model to simulate the variation of water quality concentrations in the river. By calibrating the model with water quality data collected from the selected river blocks, the simulated results of dissolved oxygen and water temperature have good agreement with the observed data. In calibrating model, we used genetic algorithms that allowed users to find the best data set of parameters which could not be measured from field measurement and experiments or analyzed simply by a user. Results of the water quality model are helpful for management, protection, and improvement of the Tatara River water quality.

Keywords: Water quality in river, modeling, water temperature, dissolved oxygen, genetic algorithm

INTRODUCTION

The Tatara River basin shown in Fig.1 is located in Fukuoka prefecture, Japan. The main stem of this river is roughly 21.5km in length and flow generally from east to west, starting in the mountainous area of Sasaguri Town and Hisayama Town, and finally discharging into the Hakata Bay –Sea of Genkai. The river has an average width of about 3m at upstream part and about 30m at downstream. The total catchments area is $101.98km^2$.

The river receives water from various sources such as non-point sources in the catchment from agricultural field slots, from both urban and non-urban areas and so on. Therefore its water quality depends largely on a number of conditions such as geology and soil types, land use, streamflow regime. Because of human, agricultural and other economic activities in the catchment, the water quality in the river has become a cause for public concern. Therefore, understanding the properties of water quality parameters affected by different sources of pollutants is very important for assessment of river water quality. On the other hand, developing a comprehensive river water quality model is necessary in water management.

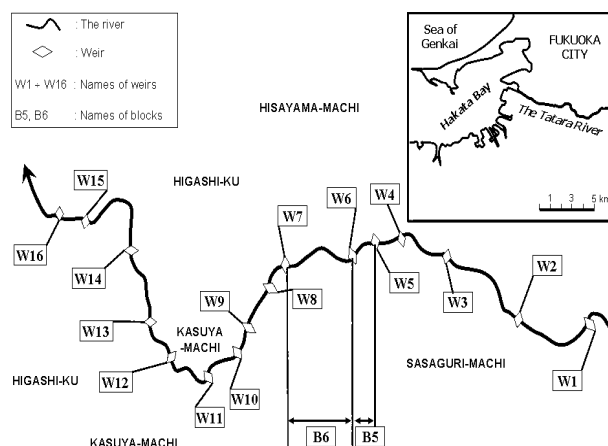There are a total of 16 weirs numbered from W1 to W16 (see Fig. 1) across the river. And along the river,

Fig. 1 Map showing the Tatara River and the selected river blocks

there are 19 intakes used for irrigation purpose and domestic uses. The river received waste water from residential areas, agricultural drainage, and rain-drainage water at 27 points. In this study, the Tatara River was divided into 15 blocks numbered from B1 to B15 (see Fig. 1). Each river block is formed by a river segment between two weirs.

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DATA COLLECTION AND ANALYSIS

Two different types of data collection were conducted; the first one is the spatial variation of water quality along the Tatara River, and another one is the temporal variation of water quality at the river blocks in order to find out the effects of different receiving sources on the river water quality. Water quality parameters such as water temperature, dissolved oxygen, pH, conductivity, turbidity, chloride ion, nitrate ion were measured directly in-situ by a portable Horiba multi-probe W-23XD. Two other parameters, total phosphorus (T-P) and total nitrogen (T-N), were estimated by an absorption-metric method using T-N-P definition equipment (HC-100). Hydraulic and meteorological data were also measured at the same time and same locations of water quality measurements.

NUMERICAL MODEL

Mass Transport Equation

The basic equation is the one-dimensional advection-dispersion mass transport equation, which is numerically integrated over space and time for each water quality constituent. For any constituent (C), this equation can be written as:

$$\frac{\partial M}{\partial t} = \frac{\partial(A_x dx C)}{\partial t} = \frac{\partial\left(A_x D_x \frac{\partial C}{\partial x}\right)}{\partial x} dx - \frac{\partial(A_x \bar{u} C)}{\partial x} dx \quad (1)$$
$$+ \left(A_x dx\right)\frac{dC}{dt} + S$$

where $M = A_x dx C$ = mass (M), t: time (T), C: concentration of water quality constituent (M L^{-3}), A_x: cross-sectional area (L^2), D_x: dispersion coefficient (L^2 T^{-1}), $\bar{u}$: mean velocity at the calculated cross-section (L T^{-1}), S: external sources or sinks (M T^{-1}); units M: Mass, L: Length, T: Time.

The left-hand side of Eq. (1) represents the time rate of change in constituent concentration. The term on the right-hand side represent dispersion, advection, constituent changes (reactions and interactions), and external sources/sinks, respectively.

Numerical Algorithm

Spatial derivatives of the dispersion, advection terms, and temporal derivative of C were expressed in the approximate expression of the finite difference method (Mitchell et al. 1985) using explicit procedure.
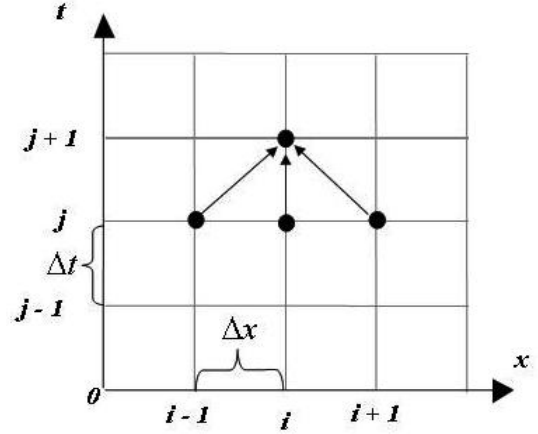

Fig. 2 Geometrical illustration of the finite difference scheme

The finite difference scheme is formulated by considering the constituent concentration, C, at four points as shown in Fig. 2. Three points are required at time j to approximate the spatial derivatives. The temporal derivative is approximated at time step $j+1$.

Equation (1) can be written in finite difference form in two steps. First, the advection and dispersion terms are differentiated once with respect to x, giving:

$$\frac{\partial C_i}{\partial t} = \frac{1}{A_x}\left(A_x D_x \frac{\partial^2 C}{\partial x^2} + A_x \frac{\partial C}{\partial x}\frac{\partial D_x}{\partial x} + D_x \frac{\partial C}{\partial x}\frac{\partial A_x}{\partial x}\right)$$
$$- \frac{1}{A_x}\left(Q_x \frac{\partial C}{\partial x} + C_x \frac{\partial Q_x}{\partial x}\right) + \frac{dC_i}{dt} + \frac{S_i}{A_i \Delta x} \quad (2)$$

where Q_x is discharge (L^{3}T^{-1}).

Secondly, expressing the spatial derivative of the dispersion terms in finite difference and thence the time derivative of C in finite difference. There results:

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = \left[\frac{A_i^j D_{xi}^j\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right)}{A_i^j \Delta x^2}\right.$$
$$+ \frac{A_i^j\left(C_{i+1}^j - C_i^j\right)\left(D_{xi+1}^j - D_{xi}^j\right)}{A_i^j \Delta x^2}$$
$$\left.+ \frac{D_{xi}^j\left(C_{i+1}^j - C_i^j\right)\left(A_{i+1}^j - A_i^j\right)}{A_i^j \Delta x^2}\right] \quad (3)$$
$$- \frac{Q_i^j\left(C_{i+1}^j - C_i^j\right) + C_i^j\left(Q_{i+1}^j - Q_i^j\right)}{A_i^j \Delta x}$$
$$+ P_i^j$$

where P_i^j is total of internal and external sources or sinks.

In this equation, all of parameters at time step j are known, and at $j+1$ is unknown (see Fig. 2). Constituent concentration at time step $j+1$ of spatial element i, C_i^{j+1}, can be obtained by:

$$C_i^{j+1} = C_i^j + M_i^j - N_i^j + P_i^j \qquad (4)$$

where

M: Dispersion term

$$M_i^j = \frac{\Delta t}{A_i^j \Delta x^2} \left\{ A_i^j D_{xi}^j \left[\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j \right) \right. \right.$$
$$\left. + \left(D_{xi+1}^j - D_{xi}^j \right) \left(C_{i+1}^j - C_i^j \right) \right] \qquad (5)$$
$$\left. + D_{xi}^j \left(C_{i+1}^j - C_i^j \right) \left(A_{i+1}^j - A_i^j \right) \right\}$$

N: Advection term

$$N_i^j = \frac{\Delta t}{A_i^j \Delta x} \left[Q_i^j \left(C_{i+1}^j - C_i^j \right) \right.$$
$$\left. - C_i^j \left(Q_{i+1}^j - Q_i^j \right) \right] \qquad (6)$$

Reaction, interactions and source/sinks terms

The differential equation used for description of the rate of change in dissolved oxygen is shown in Eq. (7), each term represents a major source/sink of oxygen.

$$\frac{dO}{dt} = K_1 \left(O_S - O \right) + \left(\alpha_1 \mu - \alpha_2 \gamma \right) A$$
$$- K_2 L - \frac{K_3}{h} - \alpha_3 \beta_1 N_1 - \alpha_4 \beta_2 N_2 \qquad (7)$$

where O is the concentration of dissolved oxygen (mg/l), O_S is the saturation concentration of dissolved oxygen at the local temperature and pressure (mg/l), K_1 is the reaeration rate in accordance with the Fickian diffusion analogy (1/day), K_2 is carbonaceous BOD de-oxygenation rate (1/day), K_3 is sediment oxygen demand rate (g/m²-day), α_1 is the rate of oxygen production per unit of algal photosynthesis (mg-O/mg-A), α_2 is the rate of oxygen uptake per unit of algal respired (mg-O/mg-A), α_3 is the rate of oxygen uptake per unit of ammonia nitrogen oxidation (mg-O/mg-N), α_4 is the rate of oxygen uptake per unit of nitrite nitrogen oxidation (mg-O/mg-N), μ is algal growth rate (1/day), γ is algal respiration rate (1/day), β_1 is ammonia oxidation rate coefficient (1/day), β_2 is nitrite oxidation rate coefficient (1/day), A is algal biomass concentration (mg/l), L is concentration of ultimate carbonaceous BOD (mg/l), h is mean stream depth (m), N_1 is ammonia nitrogen concentration (mg/l), and N_2 is nitrite nitrogen concentration (mg/l). In this study, since data points were not so dense and the experiment periods were not long enough, some parameters used in the calculation of interactions and sources/sinks terms of DO simulation were chosen experientially from previous research

(Chapra 1997), or defined using genetic algorithm, which will be mentioned later on.

The source term for water temperature can be defined by:

$$TS = \frac{H_{sn} + H_{an} - \left(H_b \pm H_c + H_e \right)}{\rho c_p h} \qquad (8)$$

where TS is source term, H_{sn} is net short-wave solar radiation flux (kW/m²), H_{an}: net long-wave atmospheric radiation flux (kW/m²), H_b: outgoing long-wave back radiation flux (kW/m²), H_c: conductive energy flux passing back (kW/m²), H_e: energy loss by evaporation (kW/m²), ρ: density of water (kg/m³), c_p: specific heat capacity of water (kJ/kg °C), h: mean water depth (m).

Dispersion Coefficient

Dispersion is basically a convective transport mechanism. The term "dispersion" is generally used for transport associated with spatially averaged variation, as opposed to "diffusion", which is reserved for transport that is associated primarily with time-averaged velocity fluctuations. The first predictive equation for the longitudinal dispersion coefficient is derived by Taylor (Hirsch 1988) for a long straight pipe. Some investigators after that have attempted to apply Taylor's expression to stream flow, and obtained only approximate results. Elder, in his researches in 1959 (Brown and Barnwell 1987), assumed that only the vertical velocity gradient was important in stream flow and developed an expression analogous to Taylor's expression, as follow:

$$D_x = 3.82 K n u h^{5/6} \qquad (9)$$

where D_x is longitudinal dispersion coefficient (m²/s), K is dispersion constant, n is Manning's roughness coefficient, u is mean velocity of the river at being calculated cross-section (m/s), h is mean water depth (m).

A comparison between the simulated results and measured data was done to find the best value of dispersion coefficients.

Solution for Inflows

For cross section between river and a branch that flows into the river, the concentration of constituent can be defined as:

$$C = \frac{Q_r C_r + Q_{br} C_{br}}{Q_r + Q_{br}} \qquad (10)$$

where Q_r is discharge of the river, C_r is concentration of the constituent in the river before the junction, Q_{br} is discharge of the inflow, and C_{br} is concentration of the constituent in the inflow.

MODEL CALIBRATION USING GENETIC ALGORITHM (GA)

GA is a prominent and powerful optimization technique that has been applied successfully in many disciplines. It is a robust search technique that is based on concepts of natural selection and genetics. For this reason, the terminology used in GA is borrowed from genetics.

Every model has its own model parameters. According to the genetics terminology, each model parameter is a gene, while a complete set of model parameters is a chromosome.

Each GA run consists of a number of generations with constant population size of several model parameters sets. The process of GA begins with an initial population of a user-defined number of model parameter variables, of which values were chosen at random or using a pre-defined rule, within a specified parameter range. Each model parameter set is then evaluated by an objective function to yield its fitness value. The second and subsequent generations are formed by combining model parameter sets with high fitness value from the previous (or parent) population using selection and sampling, crossover and mutation operations, to produce successively fitter model parameter sets or offspring. The

selection and sampling operation favors those parent parameter sets with high fitness value to those of lower fitness value in producing offspring. The crossover operator exchanges model parameter values from two randomly selected parent model parameter sets to produce a new parameter set for the current population. The mutation operator adds variability to randomly selected model parameter sets by altering some of the values randomly. Several generations are considered in one GA run, until the convergence of data is achieved.

In this study, a GA program was developed and applied. This program based on the principles of GA (see Fig. 3) and using the reciprocal of the root mean square error of the difference between the model predictions and the observed data as a fitness function.

Parameter sets needed to be optimized by GA program here were the parameters in the sources term equations mentioned above, which could not be measured from field measurement and experiments or analyzed simply by a user. For example, in Eq. (7), a set of 6 parameters related to reaeration (K_1), algal activities (α_1, α_2, μ), ammonia nitrogen oxidation (α_3, β_1) will be optimized by GA program. Several model runs have been done to find out the best values of GA operators which can be used to generate an optimal data set of these 6 parameters.

GA Operator Selection

Search space

Values of search space (see Table 1 below) were referred to QUAL2E model (Brown 1987). Actual rates were data that already defined at a specific river segment and will be used for finding the best operator set of GA program.

Fitness functions

A fitness function is the function that will be used to calculate the fitness of parameter set. In this study, Root Mean Squared Error (RMSE) equation was considered. The fitness was determined as the reciprocal of the root mean squared error of the difference between the model predictions and the observed data for water quality constituent (Pelletier et al. 2006) as shown in Eq. (11).
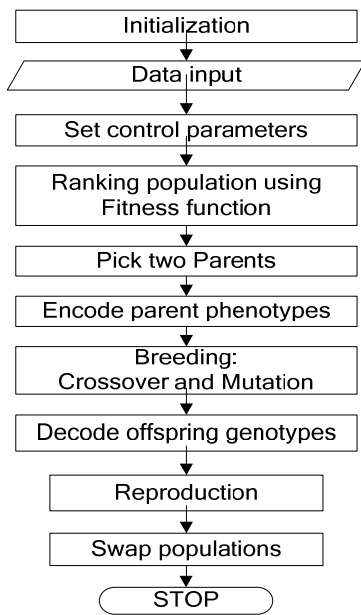

Fig. 3 Illustration of GA performance

Table 1 Search space used for GA optimization

Parameter	Search Space	Actual rate
α_1	1.710 - 1.820	1.790
α_2	1.590 - 1.630	1.615
α_3	3.800 - 4.100	4.000
β_1	0.930 - 1.040	1.000
K_1	0.000 - 1.100	0.500
μ	0.970 - 1.005	1.000

$$F = \left(\sum_{i=1}^{n} w_i \right) \left(\sum_{i=1}^{n} \frac{1}{w_i} \left(\frac{\dfrac{\sum_{j=1}^{m} O_{i,j}}{m}}{\left(\dfrac{\sum_{j=1}^{m} (P_{i,j} - O_{i,j})^2}{m} \right)^{1/2}} \right) \right) \qquad (11)$$

where: F = value of fitness, $O_{i,j}$ = observed value, $P_{i,j}$ = predicted value, w_i = weighting factor, m = number of pairs of predicted and observed values, and n = number of different state variables included in the reciprocal of the weighted normalized RMSE.

Population size and number of generations

Forty different population sizes from 25 to 220 with increasing interval +5 were tested. The number of generations used for all these population sizes were set at 250, which is big enough to get convergence of model data and not consume much computer time. We found that the model parameters converged with the population sizes ranging between 120 and 130, while they did not

converge with other population sizes. The best values of number of generation range from 132 to 140. In this step, initial values chosen for rate of crossover and mutation are 0.85 and 0.01, respectively. From the results, the population size of 125 with 135 generations was chosen as the 'optimum' population size and the number of generations, respectively, and was used in subsequent investigations.

Crossover and mutation rates

Since these two rates simultaneously determine the rate of convergence of model parameters, they should be tested together. Several combinations of rates of crossover and mutation were chosen and tested in order to find out the optimal set of GA operators. Varying increments within the range 0.0025–0.03 were considered for mutation rate with increasing constant interval of 0.0025, while constant interval of 0.05 was considered for crossover rate within the range 0.40–0.90.

By comparing the values of six parameters with the actual values as shown in Table 1, some best ranges of result were found as marked by the ellipse shapes in Fig. 4. From this result, the best combination of crossover probability (*Pc*) and mutation probability (*Pm*) were designed in ranges of *Pc* from 0.74 to 0.76, *Pm* from 0.0272 to 0.0276, and *Pc* from 0.58 to 0.62, *Pm* from 0.0224 to 0.0227.

In order to find the optimal set of GA operators, one more coefficient called coefficient of variation (*CV*) was checked. *CV* coefficient calculates the differences between calculated values of each parameter and the corresponding mean values, respectively.

Most of parameters have convergences with values of *Pc* ranged from 0.55 to 0.63 and *Pm* ranged from 0.022 to 0.023. While checking convergences of mean values of parameter, comparing with combinations of *Pc* and *Pm* found that the best combination of crossover and mutation rates are defined, with *Pc* ranged from 0.58 to 0.62 and *Pm* from 0.0224 to 0.0227 (see Fig. 4).

The optimal set of GA operators

The optimal set of GA operators was obtained with the number of generation being 135, population size of 125, crossover rate of 60% and mutation rate of 2.25%.

RESULTS AND DISCUSSION

Properties of Water Quality Parameters

Typical properties such as DO, pH of the Tatara River water quality found from collected data as follows:
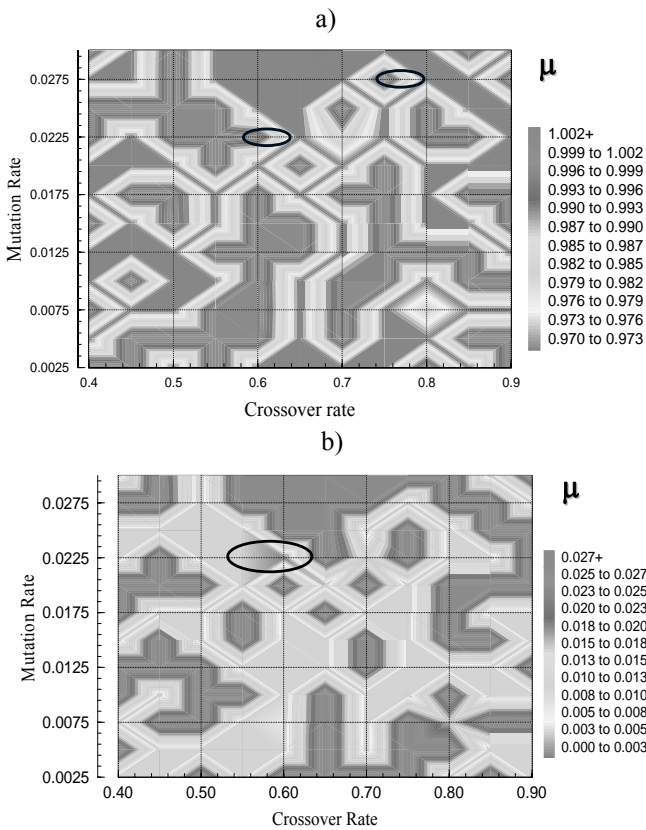

Fig. 4 Example of estimation of *Pc* and *Pm* combination based on: a) Real value; b) Coefficient of variation
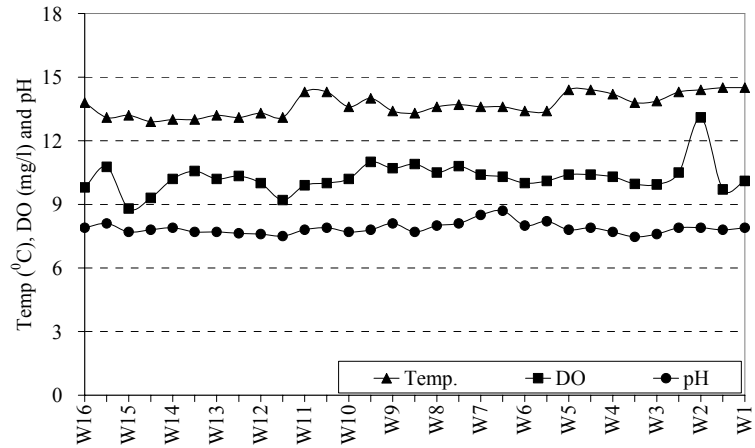
Fig. 5 Variation of water temperature, DO and pH along the river on 27 November 2003
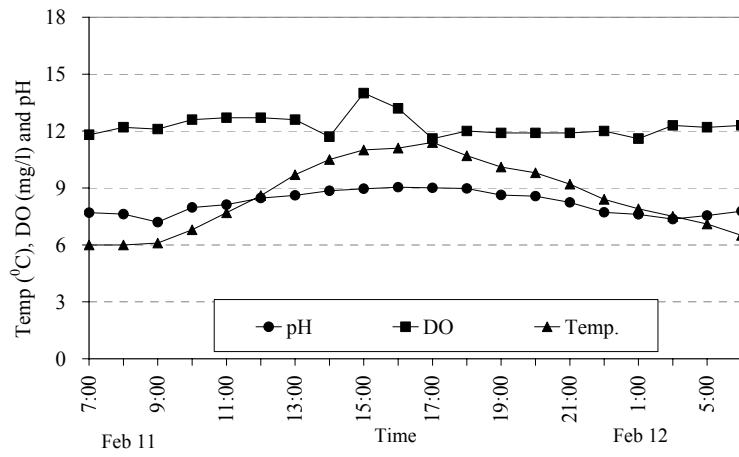
Fig. 6 Variation of water temperature, DO and pH at block B8 in 24 hours from 11 Feb 2004 to 12 Feb 2004
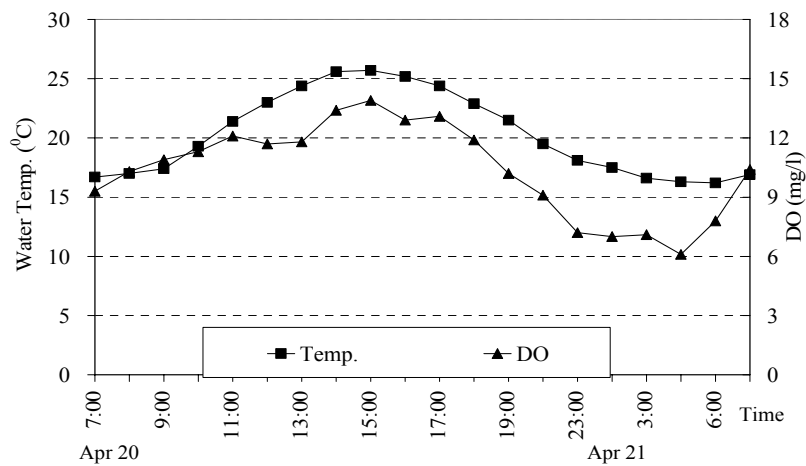
Fig. 7 Variations of DO and water temperature at point B5-1 (in Block B5)
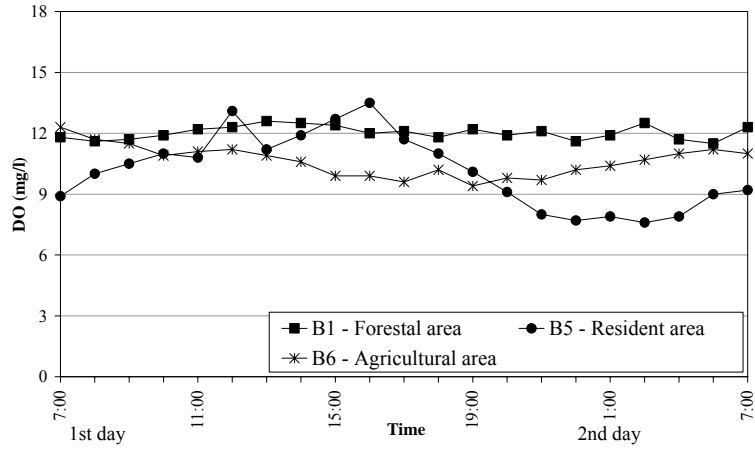
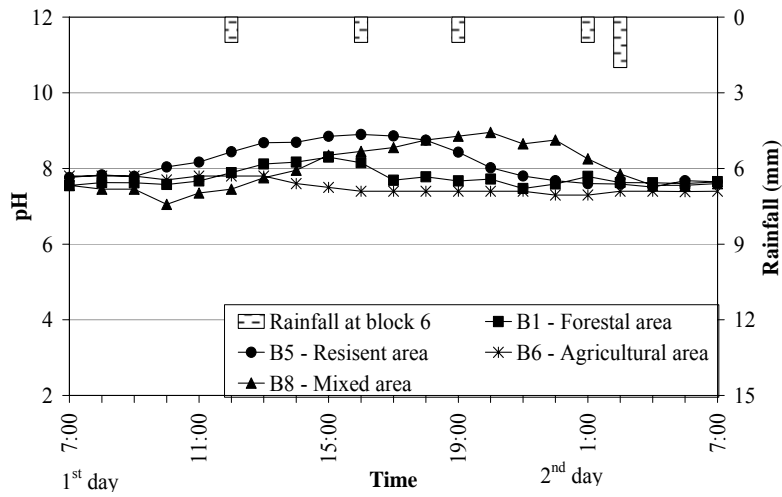Fig. 8 Variation of DO measured at different blocks

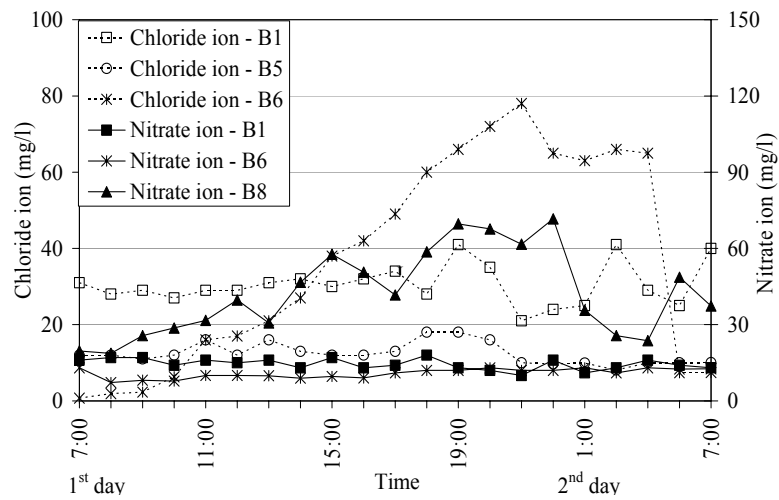Fig. 9 Variation of pH measured at different blocks

Fig.10 Variation of ions measured at different blocks

Table 2 Japan standard for water quality parameters

Class	Water use	Standard	
		pH	DO
AA	Water supply class 1, conservation of natural environment, and uses listed in A-E	6.5-8.5	7.5 mg/l or more
A	Water supply classes 2,fishery class 1, bathing, and uses listed in B-E	6.5-8.5	7.5 mg/l or more
B	Water supply classes 3, fishery class 2, bathing, and uses listed in C-E	6.5-8.5	5 mg/l or more
C	Fishery class 3, industrial water class 1, and uses listed in C-E	6.5-8.5	5 mg/l or more
D	Industrial water class 2, agricultural water, and uses listed in E	6.0-8.5	2 mg/l or more
E	Industrial water class 3 and conservation of the environment	6.0-8.5	2 mg/l or more

(Source: Ministry of the Environment - Japan)

- Most of water quality parameters in the Tatara River satisfied the Japan Criteria for fishery and agricultural supply and conservation of natural environment (see Figs. 5, 6 and Table 2).

-Normally, the ability of water to hold oxygen in solution is inversely proportional to water temperature. In this river, it is proportion to water temperature (see Fig. 7) both in daytime and nighttime, because of the photosynthesis phenomenon of aquatic plants in river water and turbulent states of river flow in the daytime.

-Rapidly moving (in a forestal area - block B1) water often contains a high level of dissolved oxygen (see Fig. 8). The most complex and lowest values of DO were found in the block which receives wastewater from domestic uses (block B5).

-pH in a flooding period was lower than that in a dry period, because of the acidity of rainwater. This parameter was high in block that receives much of wastewater from resident areas (see Fig. 9).

Concentrations of some ions such as nitrate (NO_3^-) and chloride (Cl^-) in the Tatara River were small. Their values changed largely in different sources of receiving water (see Fig. 10). The concentration of ions in river water increased with growing of wastewater sources from agricultural area (block B6) or fixed area (Block B8).

Main parameters used in this model are shown in Tables 3 and 4.

Table 3 Parameters used for simulations of temperature

Parameter	Unit	Block	
		B5	B6
River length	m	425.00	400.00
Sub-interval of river length	m	25.00	25.00
Time period	hour	24.00	24.00
Time step	second	1.00	1.00
Elevation of the site	m	49.70	49.70
Latitude	degree	33.62	33.62
Longitude of local meridian	degree	130.51	130.51
Coefficient ε	-	1.00	1.00
Sky covered decimal fraction	-	0.50	0.70
Local barometric pressure	mmHg	760.48	760.48
River depth	m	0.25	0.30
Specific weight of water being evaporated	kg/m^3	998.48	998.48
Specific heat capacity of water	kJ/kg-°C	4.19	4.19
Solar constant	kW/m^2	1.38	1.38
Atmospheric radiation reflectivity	-	0.03	0.03

Table 4 Parameters used for simulations of DO

| Parameter	Unit	Block	
		B5	B6
Reaeration rate (K_1)	1/day	0.50	0.50
Carbonaceous BOD de-oxygenation rate (K_2)	1/day	3.40	3.49
Sediment oxygen demand rate (K_3)	g/m^2-day	10.75	10.75
The rate of oxygen produced by algal photosynthesis (α_1)	mg-O /mg-A	1.79	1.79
The rate of oxygen uptake per unit of algal respired (α_2)	mg-O /mg-A	1.60	1.60
The rate of oxygen uptake per unit of ammonia nitrogen oxidation (α_3)	mg-O /mg-N	4.00	4.00
The rate of oxygen uptake per unit of nitrite nitrogen oxidation (α_4)	mg-O /mg-N	1.07	1.07
Algal growth rate (μ)	1/day	0.98	0.98
Algal respiration rate (ρ)	1/day	0.25	0.25
Ammonia oxidation rate coefficient (β_1)	1/day	1.00	0.94
Nitrite oxidation rate coefficient (β_2)	1/day	1.09	0.96
Mean depth of stream	m	0.25	0.30

a)

b)
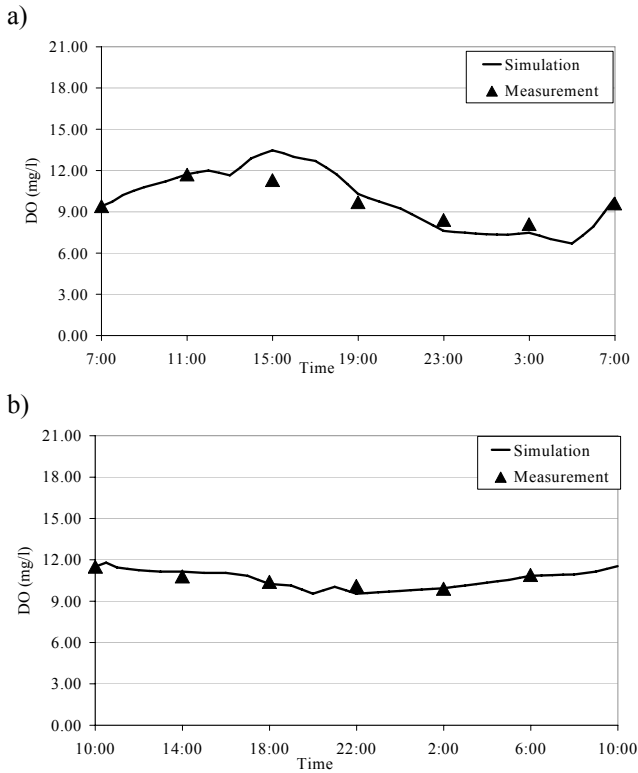
Fig. 11 Variation of DO simulations at: a) Block B5 and b) Block B6
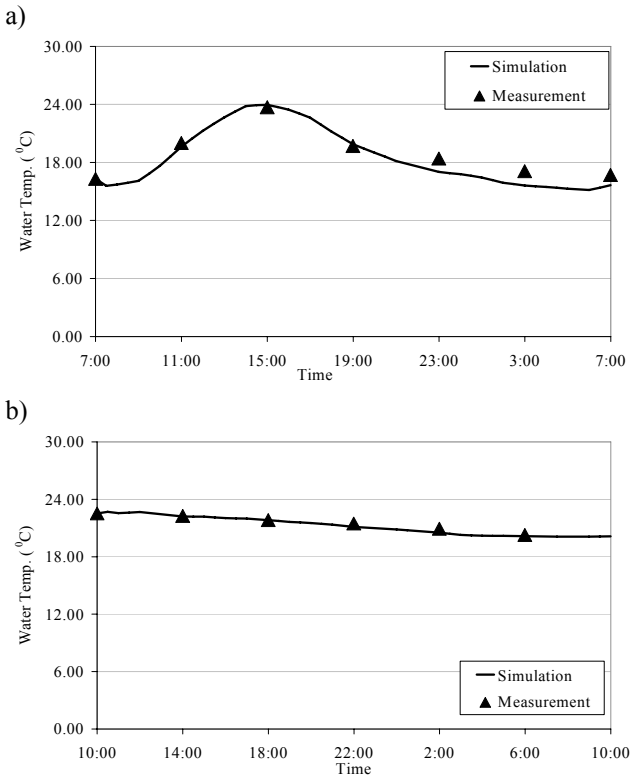
a)

b)

Fig. 12 Variation of water temperature simulations at: a) Block B5 and b) Block B6

For simulating water temperatures, the model considers all of terms in the dispersion-advection mass transport equation such as dispersion, advection and sources or sinks terms. For DO, all of these terms were also calculated. Six parameters mentioned above were calibrated using the GA program. Other remaining coefficients were chosen empirically based on parameters simulated for some other similar rivers (Brown 1987). This model also allows users to try values of dispersion constant K in order to find the optimal simulation for each water quality parameter at different river blocks.

Values of dispersion constant $K= 30000$ in block B5 and $K= 6500$ in block B6 were found for simulations of water quality parameters. Results from simulations applied to river blocks along the Tatara River showed the dependences of dispersion constant on hydraulic properties such as flow velocities, water depth, surface width, and river bottom conditions.

Figures 11 and 12 show the comparison between the simulated and measured data. Results of the model showed that the simulated results had good agreement with the observed data. Both of DO and water temperature at block B5 changed larger than at block B6. Data at block B6 was collected at the time of higher water temperature but it was a rainy day (see Fig. 9) and, therefore, variation of water temperature was not large. On the contrary, temperature at block B5 was higher at daytime but lower at nighttime. For DO, as mentioned above, variation of DO had the same trends with water temperature; it was more stable at block 6. This reason also caused the big value of dispersion constant K found at block B5, while it was small at block B6.

CONCLUSIONS

Field-measurements for water quality were conducted along the Tatara River and at some specific river blocks which received different pollutant sources. Collected data included the most important water quality parameters as well as hydraulic and meteorological data. From these data, the variations of water quality, the dependence of water quality on other factors such as conditions of hydrology, hydraulics, meteorology, and especially, the variations of river water quality affected by different pollutant sources, were understood.

A one-dimensional water quality model was developed and applied for simulating water temperature and dissolved oxygen concentration at several specific river blocks along the Tatara River. Results of the model showed that the simulated results had good agreement with the observed data. However, the model has some

limitation when dealing with problems having complex variations and dependences. In order to face with this difficulty, a GA model was developed and applied to find the optimal data sets for water quality parameters. It can be concluded that calibration using GA program was found to be better in comparison to the traditional calibration. The advantages of using GA in model calibration are in computational time saving and getting the best data set from large useable data range.

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