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Building a Mathematical Model for Simulating River Water Quality, a Case of Study Applied to the Tatara River in Fukuoka City

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From an advection–dispersion equation based on the mass conservation law, I developed a theoretical model for simulating the alteration of the Tatara river's water quality according to time. This equation has been solved for water quality variables by method of finite–difference approximations for the derivatives in the equation. To solve this equation effectively, an algorithm has been developed and a software program has been coded in Fortran language 90 (Nyhoff and Leestma, 1997, 1999) to implement this algorithm. As a case of study, the Tatara river's water quality parameters, hydraulic parameters such as discharge, velocity as well as cross–sections of the river and meteorological data of the river area have been observed and used as initial and boundary conditions for the model. The calibration of the model has been made by the trial–by–error method to find a reasonable dispersion constant that helps to obtain an optimal agreement between the model calculations and the set of observed data.

INTRODUCTION

It is well known that rivers and streams play an important part in life. On the one hand, they are main sources of water supply for various purposes such as farming and industry, and they are also receiving sources of waste loadings from activities made by human on the other hand. With an increase of economic activities, rivers and streams seem to burden more and more waste loadings which make their water quality become more and more degraded (Haygraph and Jarvis, 2002). In turn, their water quality directly affects activities using the waters such as farming and fishery, as well as causing problems to the regional environment they flow through. Therefore, understanding the response of their water quality to external waste loadings as well as the alteration of water quality parameters has a great significance in examining and analysing the quality of water bodies in general and river water quality in particular. One of the effective ways to gain an insight into the change of water quality is to apply mathematical models in simulating its response to external waste loadings. Up till now, there are some existing water–quality models such as the QUAL2E (Brown and Barnwell, 1987), the Water Quality Analysis Simulation Program (WASP) (US EPA, 1985; Ambrose *et al.*, 1993), CE–QUAL–W2 (Cole and Buchak, 1995), the Branched Lagrangian Transport Model

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(BLTM) (Jobson, 2001). However, the main concern of using the existing models is that they are not the best appropriate for some particular cases of study due to the complex operation of the programs or too much requirement for inputs to the programs. Complex water quality models such as CE–QUAL–W2 require many types of data (Rounds and Wood, 2001). With an effort to contribute to the comprehensive understanding of river water quality, this research has been made on the mathematical bases to build a suitable model for simulating river water quality. Then, the model is applied to simulate the water quality of the Tatara river as a particular case of study.

MATERIALS AND METHODS

Study area

The Tatara river basin is located in Fukuoka prefecture in the north–western part of Kyushu Island. The main flow of the Tatara river is formed by three big distributaries: the Tatara river, the Umi river which joins the Tatara river at the distance of 1.5 km from river mouth, and the Hisahara river with the confluence is 5.2 km from river mouth. The main stem of the Tatara river is roughly 21.5 km in length and flows generally from east to west, starting in the mountainous area of Sasaguri town and Hisayama town, and finally discharging into the Hakata Bay – Japan Sea. The river has an average width of about 3 m at head reach and about 30 m at downstream. Along the Tatara river, there are many weirs constructed across the river.

In this research, a segment of the river is selected from a big weir at Tanotsu, which is about 3.2 km from the river's mouth, to upstream of the Tatara river. This segment has a total length of about 18.3 km, and flows through Sasaguri town, Hisayama town and Kasuya town in Fukuoka City.

The total catchment's area is 101.98 km^2, in which 73.23 km^2 is mountainous and forestal area, 15.93 km^2 is residential area, and 9.96 km^2 is paddy fields and agricultural area. There are total 16 weirs across the river, 27 outtake points and 19 intake points along this segment of the river. Almost intakes are used for the purpose of irrigation, some of them supply water for domestic uses through treatment stations. The sources of

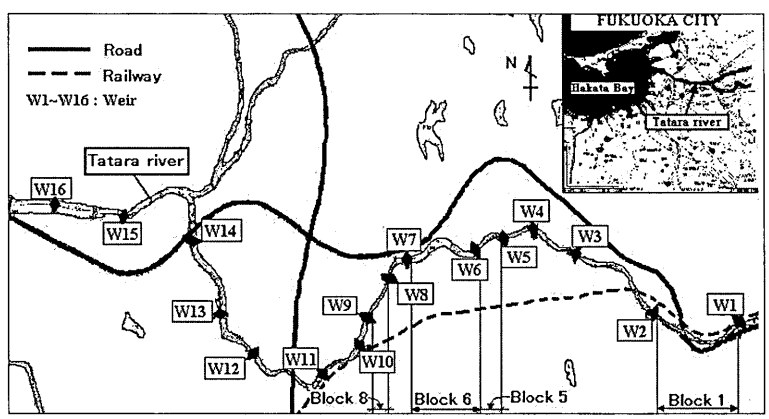

Fig. 1. Location of the studied blocks in Tarara river–Fukuoka, Japan

receiving water are different, including waste water from residential area, agricultural area, drainage of rain water, etc.

For the purpose of the study, this segment of the river is divided into 16 blocks intercepted by weirs at two ends of each block as can be seen in Fig. 1.

Mathematical base of the model and data requirement

One–dimentional equation for river water quality

As can be seen from Fig. 2, if the dispersion component is not taken into account, we can write a mass balance for a river's element with the lengh of Δx as follows :

$$\frac{\partial Vc}{\partial t} = J_{in} - J_{out} \pm reaction + s \tag{1}$$

Where V is volume of the element $(=A_r \Delta x)$, c is constituent concentration, A is the mean cross–sectional area, b is the mean river width, h is the mean depth, J_{in} and J_{out} are fluxes of mass in and out of the element due to transport, *reaction* is gain or loss mass within the element due to reaction $(=V\frac{dc}{dt})$, s is external sources or sinks of the constituent.

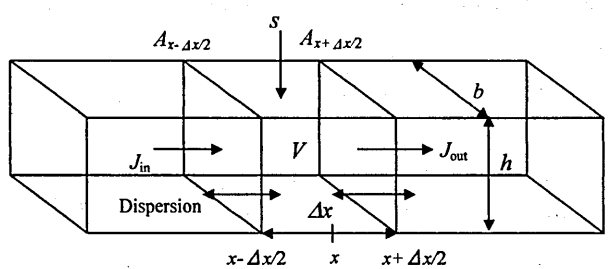

Fig. 2. A mass balance for a differential element of length Δx.

When the dispersion component is taken into account, based on Fick's first law, J_{in} and J_{out} can be calculated as follows :

$$J_{in} = [A(Uc - E\frac{\partial c}{\partial x})]_{x-\Delta x/2} \tag{2}$$

$$J_{out} = [A(Uc - E\frac{\partial c}{\partial x})]_{x+\Delta x/2} \tag{3}$$

Where E is turbulent diffusion, and U is average velocity of the flow.

Using Taylor expansion gives :

$$J_{in} = [A(Uc - E\frac{\partial c}{\partial x})]_{x-\Delta x/2} = A(Uc - E\frac{\partial c}{\partial x})_x - \frac{\partial}{\partial x}[A(Uc - E\frac{\partial c}{\partial x})]_x \times \frac{\Delta x}{2} \tag{4}$$

$$J_{out} = [A(Uc - E\frac{\partial c}{\partial x})]_{x+\Delta x/2} = A(Uc - E\frac{\partial c}{\partial x})_x + \frac{\partial}{\partial x}[A(Uc - E\frac{\partial c}{\partial x})]_x \times \frac{\Delta x}{2} \tag{5}$$

Substituting (4) and (5) into (1) yields

$$\frac{\partial Vc}{\partial t}=\frac{\partial}{\partial x}(A_r E\frac{\partial c}{\partial x})\Delta x-\frac{\partial}{\partial x}(A_r Uc)\Delta x\pm V\frac{dc}{dt}+s \tag{6}$$

The left side of the equation (6) can be written as follows :

$$\frac{\partial Vc}{\partial t}=V\frac{dc}{dt}+c\frac{dV}{dt} \tag{7}$$

If we assume the flow in the stream is steady ($\frac{\partial Q}{\partial t}=0$) then the term $\frac{dV}{dt}=0$ and the equation (6) becomes :

$$\frac{\partial c}{\partial t}=\frac{\partial(A_r E\frac{\partial c}{\partial x})}{A_r\partial x}-\frac{\partial(A_r Uc)}{A_r\partial x}+\frac{dc}{dt}+\frac{s}{V} \tag{8}$$

In principle, the equation (8) can be applied to any water quality parameter. Within this research, two main parameters are chosen to illustrate the methodology namely water temperature (T), and dissolved oxygen (DO).
In a similar way to the equation (8), we can write equations for DO and T as follows :

$$\text{For } DO: \quad \frac{\partial DO}{\partial t}=\frac{\partial(A_r E\frac{\partial DO}{\partial x})}{A_r\partial x}-\frac{\partial(A_r UDO)}{A_r\partial x}+\frac{dDO}{dt}+\frac{s}{V} \tag{9}$$

$$\text{For } T: \quad \frac{\partial T}{\partial t}=\frac{\partial(A_r E\frac{\partial T}{\partial x})}{A_r\partial x}-\frac{\partial(A_r UT)}{A_r\partial x}+\frac{dT}{dt}+\frac{s}{\rho C_p V} \tag{10}$$

Where DO is dissolved oxygen, T is water temperature, $\frac{dT}{dt}$ in (10) is internal heat generation or loss (such as boundary friction and viscous dissipation of energy) which can be negligible because it is very small, t is time, ρ is density of water, C_p is specific heat of water, $\frac{dDO}{dt}$ in (9) refers to the changes of DO within the river volume (V) (such as the increase in DO due to photosynthesis or the decrease in DO due to decomposition of organic matters). It can be calculated as follows (Orlob, 1983) :

$$\frac{dDO}{dt}=K_2(DO_s-DO)-K_1BOD-\frac{K_4}{H}+(\alpha_3\mu-\alpha_4\rho_a)A-\alpha_5\beta_1N_1-\alpha_6\beta_2N_2 \tag{11}$$

Where K_2 is reaeration rate, DO_s is saturation concentration of dissolved oxygen. It can be calculated in following formula (APHA, 1992) :

$$\log_e DO_s=-139.34411+\frac{1.575701\times10^5}{T_a}-\frac{6.642308\times10^7}{T_a^2}+\frac{1.243800\times10^{10}}{T_a^3}-\frac{8.621949\times10^{11}}{T_a^4} \tag{12}$$

T_a is absolute temperature (K) $T_a=T+273.15$, K_1 is carbonaceous BOD deoxygenation rate, BOD is biochemical oxygen demand, K_4 is sediment oxygen demand rate, H is mean water depth, α_3 is the rate of oxygen production per unit of algal photosynthesis, μ is algal growth rate, α_4 is the rate of oxygen uptake per unit of algal respired, ρ_a is algal respiration rate, A is algal biomass concentration, α_5 is the rate of oxygen uptake per unit of ammonia nitrogen oxidation, β_1 is ammonia oxidation rate coefficient, N_1 is amonia nitrogen concentration, N_2 is nitrite nitrogen concentration.

s is external sources or sinks of the constituent. For DO, it is very small enough to neglect s. For water temperature, it is the net heat flux into the water surface, which can be calculated as follows :

$$s=H_{sn}+H_{an}-(H_{br}+H_c+H_e) \tag{13}$$

These components can be explained in the Fig. 3 below

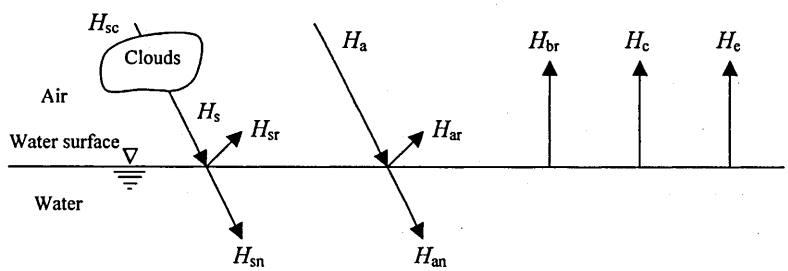

Fig. 3. Components of water surface heat exchange.

Where H_{sc} is clear-sky solar (short-wave) radiation, H_s is solar radiation at water surface, H_{sr} is reflected solar radiation, H_{sn} is net solar shortwave radiation into the water surface, H_a is atmospheric (long-wave) radiation, H_{ar} is reflected atmospheric radiation, H_{an} is net atmospheric longware radiation into the water surface, H_{br} is longware back radiation from the water surface, H_c is conductive heat flux from the water surface, H_e is evaporative heat flux from the water surface.

Calculation of the net heat flux into the water surface (s)

a) Solar shortwave radiation (H_{sn})

The net solar radiation into the water surface is the coming radiation from the sun, less that absorbed in the atmosphere, blocked by clouds and reflected at the water surface. Ryan and Harleman (1973) suggested a formula for calculating this component as follows :

$$H_{sn}=0.94\,H_{sc}(1-0.65C^2) \tag{14}$$

Where H_{sc} is the clear sky solar radiation, C is the fraction of the sky covered by clouds. The factor 0.94 accounts for average reflectance at the water surface. With the use of meteorological equipment, the term $H_{sc}(1-0.65C^2)$ can be obtained by direct measure-

ment in site, therefore:

$$H_{sn}=0.94Hs_{measured} \tag{15}$$

Where $Hs_{measured}$ is solar radiation energy directly measured by meteometer in site.

b) Atmospheric long wave radiation(H_{an})

The atmosphere itself emits longwave radiation. This component can be represented as a modification of the Stefan–Boltzmann law below :

$$H_{an}=\delta(T_{air}+273)^4(A+0.031\sqrt{e_{air}})(1-R_L) \tag{16}$$

Where δ is the Stefan–Boltzmann constant$=4.9\times10^{-3}$ J (m^2 d K^4)$^{-1}$, T_{air} is air temperature (°C), A is a coefficient (0.5 to 0.7), e_{air} is air vapor pressure (mmHg), R_L is reflection coefficient ($\approx$ 0.03).

c) Longwave back radiation from the water surface (H_{br}) (Shanahan, 1985)

$$H_{br}=5.44\times10^{-8}(T_s+273)^4 \tag{17}$$

Where T_s is water surface temperature.

d) Conductive heat flux from the water surface (H_c) (Shanahan, 1985)

$$H_c=0.60f(w)(T_s-T_a) \tag{18}$$

Where $f(w)$ is wind speed function, it defines the dependence of the transfer on wind velocity over the water surface, wind speed (w) measured at a fixed distance above the water surface. It can be calculated as follows (Roesner *et al*, 1977) :

$$f(w)=42.5+16.9\,w \tag{19}$$

Where w is wind speed, T_s is water surface temperature (°C), T_a is air temperature (°C).

e) Evaporative heat flux from the water surface (H_e) (Shanahan, 1985)

$$H_e=(1.01-9.1\times10^{-4}T_s)f(w)(e_s-e_a) \tag{20}$$

Where $f(w)$ is wind speed function, it can be calculated by the formula (19)

e_s is the saturation vapor pressure of the air at the temperature of the water surface (mmHg). It can be calculated as follows (Chapra, 1997):

$$e_s=4.596e^{\frac{17.27T}{237.3+T}} \tag{21}$$

T is air temperature, e_a is the vapor pressure at 2 meters above the water surface (mmHg). It can be calculated as follows (Chapra, 1997):

$$e_a=\frac{e_sR_h}{100} \tag{22}$$

With R_h is relative humidity.

Data requirement

To simulate the water quality of a river's block, three kinds of data are needed to collect as follows

1) Water quality data: Water temperature and *DO* are collected at two ends of each block (upstream and downstream points of each river block) and used as boundary conditions

of the model. The boundary data are measured every one hour during a daily period of 24 hours. In addition, along with the length of the river block, at some cross-sections, water temperature and *DO* are also measured and used as initial conditions for the model. The measurement is made on site by using the W-23XD multi probe (Horiba, Ltd., 2001).

2) The data of river's hydraulic characteristics: In addition to water quality parameters, the hydraulic data of the river block such as discharge (Q), velocity (V), water depth (H), wetted area (A) are needed to collect at two ends of each block and at the same locations chosen to measure water quality parameters along with each block.

3) Meteorological data of the study area: The third type of data necessary to collect is meteorological data in the study area. They are measured every 2 minutes by setting up sensors for wind direction, wind velocity, air temperature, and relative humidity.

Three types of the data above are organized in the form of data file in Fortran language 90 (Nyhoff and Leestma, 1997, 1999).

Scheme of Calculation

A numerical solution for the equations (9) and (10) can be developed by substituting finite-difference approximations for the derivatives. As shown in Fig. 4, the computational grid is used to characterize the spatial and temporal dimensions of calculated elements.

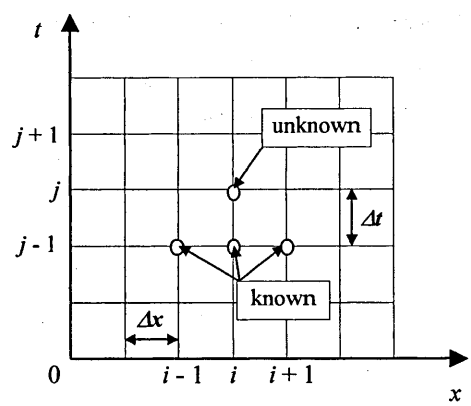

Fig. 4. A grid for calculated elements using method of finite-difference approximations.

In which t is time, x is distance of the simulated block of the river, j is time step of calculation, i is spatial step of calculation, Δx is sub-intervals of calculated distance, Δt is sub-intervals of calucated time.

The process of calculation is started at time step $j=0$. At this time, all parameters are known, and they are initial conditions of the solution. This initial conditions along with boundary conditions at ends of calculated block are inputs to calculate the value of elements at time step $j+1$. This approach is known as explicit difference approximations (Mitchell and Griffiths, 1985)

Model calibration

Calibration is the process in which one or more parameter inputs of the model are adjusted to make the model have a best fit with observed data set. In this model, the parameter chosen to calibrate is the longitudinal dispersion coefficient (E). It is calculated as a function of the river's characteristics, by the following formula (Brown Barnwell, 1987) :

$$E=3.82\times K\times n\times U\times H^{5/6} \tag{23}$$

Where E is longitudinal dispersion coefficient (m^2/s), n is channel's roughness coefficient, U is mean velocity (m/s), H is mean depth (m), K is dispersion constant.

By trial–by–error method, we can calibrate the model by adjusting the dispersion constant (K) until the results of simulation have the best fit with observed data sets.

Model application

After the scheme of calculation for the model is coded in Fortran language 90, it is applied to simulate the daily variation of water temperature and DO in 4 blocks of the Tatara river with the different characteristics as described in Table 1 below.

Table 1. Some primary characteristics of the studied blocks.

Characteristics of the block	Block			
	Block 1	Block 5	Block 6	Block 8
Mean discharge Q_{mean} (m^3/s)	0.47	0.28	1.03	3.70
Mean velocity V_{mean} (m/s)	0.58	0.28	0.50	0.54
Mean depth h (m)	0.38	0.24	0.28	0.44
Mean width b (m)	2.13	4.17	7.38	15.63
Total length L (m)	1,100	425	450	450
Regional characteristic	forestal and mountainnous area	residential area	fields and paddy fields area	mixed area.
Note	Measured on Feb. 2 & 3, 2004	Measured on Apr. 20 & 21, 2004	Measured on June 7 & 8, 2004	Measured on Feb. 11 & 12, 2004

RESULTS AND DISCUSSION

The blocks applied to simulate are sub–divided into intervals of 25m in length. The results of simulation for above blocks are expressed in Figs. 5–10 below. From the Figs.,

we can see that the daily alteration of river water temperature is directly proportional to that of air temperature and solar radiation. During a daylight, due to the increase of air temperature and solar radiation, the water temperature also increases. In contrary, at night when air temperature decreases, and solar radiation is extinct, water temperature also decreases. This can be seen clearly in Figs. 5, 6 and 8.

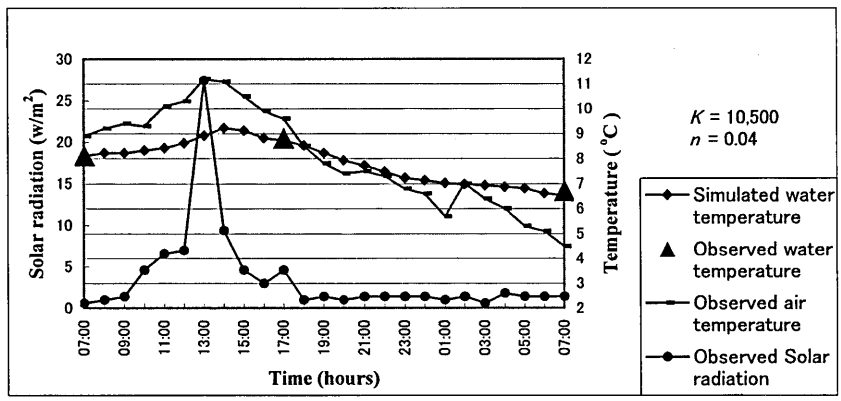

Fig. 5. The result of water temperature simulation for block 1 in relationship with solar radiation and air temperature at the point B1–2, 75 m from the upstream of block 1 (Feb. 2 & 3, 2004).

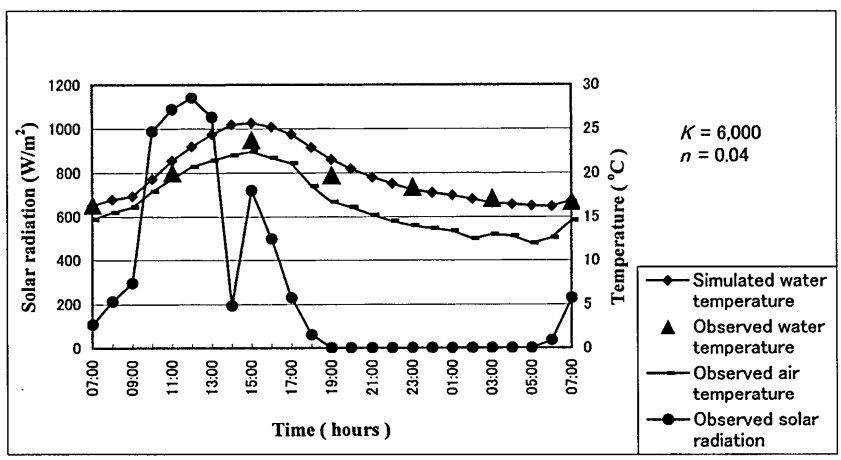

Fig. 6. The result of water temperature simulation for block 5 in relationship with solar radiation and air temperature at the point B5–3, 325 m from the upstream of block 5 (April 20 & 21, 2004).

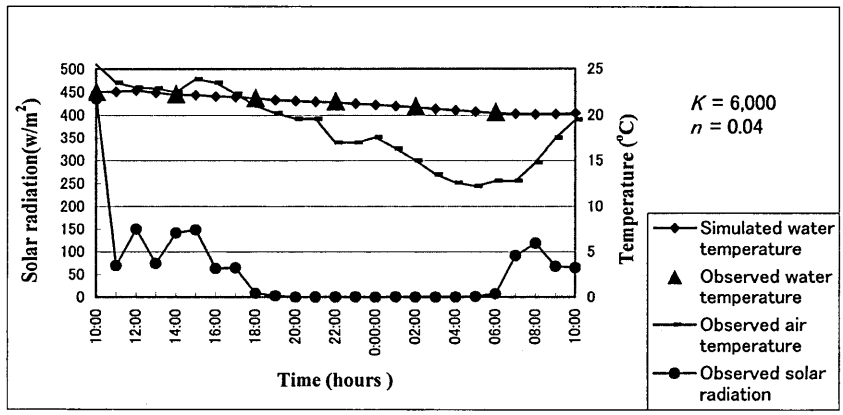

Fig. 7. The result of water temperature simulation for block 6 in relationship with solar radiation and air temperature at the point B6–2, 75 m from the upstream of block 6 (June 6 & 7, 2004).

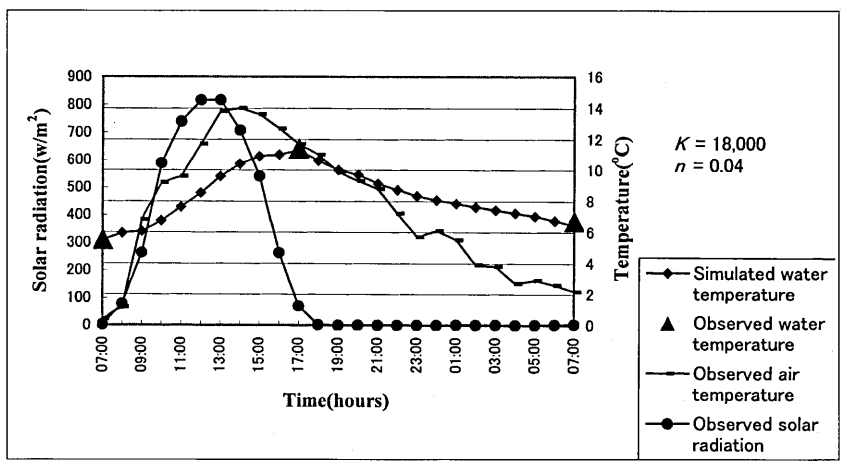

Fig. 8. The result of water temperature simulation for block 8 in relationship with solar radiation and air temperature at the point B8–2, 175 m from the upstream of block 8 (Feb. 11 & 12, 2004).

It also can be seen that solar radiation and air temperature reach at peak some hours earlier before the peak water temperature occurs. It accounts for the fact that it takes time to transfer the heat energy from solar radiation and air temperature into water.

With respect to Dissolved oxygen (*DO*), Figs. 9 and 10 show clearly that during the daylight, dissolved oxygen (*DO*) is higher than that at night. During the daylight, dissolved oxygen (*DO*) is above 10 mg/L, while it is below 10 mg/L at night. From Figs. 9 and 10, we can see that the alteration of dissolved oxygen (*DO*) seems directly proportional to

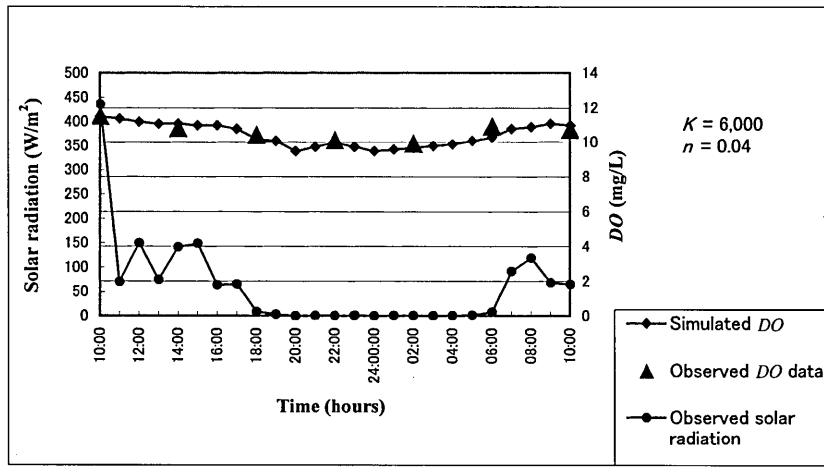

Fig. 9. The result of *DO* simulation during a daily cycle at the point B6–2, 75 m from the upstream of block 6 (June 6 & 7, 2004).

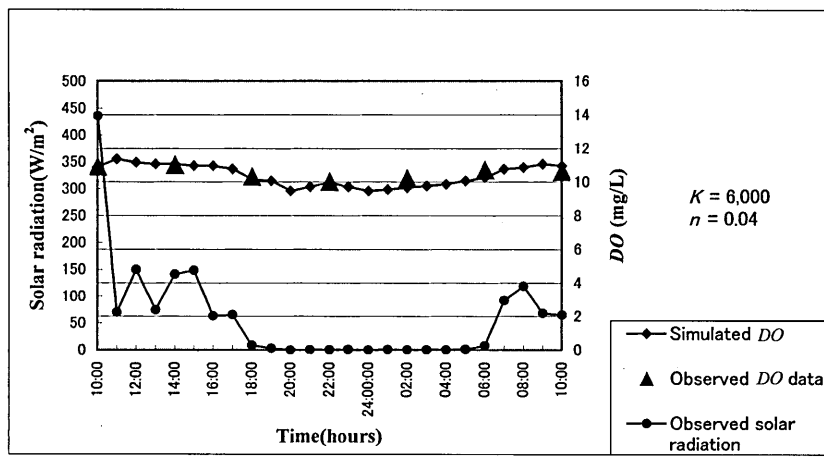

Fig. 10. The result of *DO* simulation during a daily cycle at the point B6–3, 175 m from the upstream of block 6 (June 6 & 7, 2004).

the alteration of solar radiation. From 10 o'clock to 18 o'clock, when solar radiation decreases, dissolved oxygen (*DO*) also tends to decrease. From 6 o'clock to 10 o'clock of next day, when solar radiation tends to increase, dissolved oxygen (*DO*) also increases. During the night time, when solar radiation is extinct, dissolved oxygen (*DO*) seems to be constant at below 10 mg/L. The variation of dissolved oxygen (*DO*) can be explained by the phenomenon of photosynthesis. In the river, there are some aquatic plants such as algal, during the daylight, the process of photosynthesis takes place in the water. As a

result, the process adds oxygen to water. In contrary, at night the process of respiration dominates, and it depletes dissolved oxygen (*DO*) in water.

CONCLUSION

From the results of simulation presented above, we can draw some conclusions :

In general, the results of simulation have a good fit with observed data sets. The results of calibration show that each block has a specific dispersion constant (K) :

- Block 1 : $K=10{,}500$
- Block 5 : $K=6{,}000$
- Block 6 : $K=6{,}000$
- Block 8 : $K=18{,}000$

This is obvious because there is a difference of hydraulic characteristics among blocks, it leads to the difference of longitudinal dispersion coefficient (E) among blocks. Therefore, dispersion constant (K) varies block by block to represent specific hydraulic characteristics of a block.

The model is built on the basis of some simplifying assumptions. The key assumptions of the model are :

- The flow of river is well–mixed vertically and laterally. That's why the model is one–dimensional.
- The flow of river is steady–state. It means that the flow does not vary temporally ($\frac{dQ}{dt}=0$).
- Water temperature is simulated as a function of meteorology on a scale of a daily 24–hour period.
- Characteristics of the river's bank and bed within a block chosen to simulate are uniform (the roughness of a block is uniform).

Because of some simplifying assumptions above, it is obvious that there are also some limitations in applying the model such as the model is only applicable to rivers their flow is steady–state (it is not applicable to time–variable flow). Besides, a block of the river chosen to simulate must be divided into sub–segments equal in length. Furthermore, the model is not able to simulate river's blocks with in–flows and out–flows. However, the model is being developed in an effort to include these in–flows and out–flows as well as the characteristic of time–variable flow to make the model more useful.

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