

A regionalized river water quality model calibration method based on watershed physical characteristics: application to the Cau River in Vietnam

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Article abstract

A methodology is proposed for the calibration of river water quality models on large watersheds, in the absence of intensive measurements for water quality and quantity. This methodology is based on: 1) the use of the results from a hydrological model to provide the required hydrological variables to the water quality model; 2) five assumptions for the definition of initial and boundary conditions; 3) a three-step regionalized calibration method, in which the specific characteristics of the different subwatersheds are taken into account and 4) the adjustment of some parameters in order to reproduce processes that are not explicitly represented in the model. The regionalized calibration method relies on a comprehensive study of the land use and characteristics on each subwatershed and the definition of different sets of parameters values in distinct regions. Application to the Cau River, in Vietnam, with QUAL-GIBSI, an adaptation of the QUAL2E model, showed that: *i*) calibration and validation results were significantly improved by applying regionalized calibration as compared to an initial calibration for which a single set of parameters values was used for the whole simulated river stretch and *ii*) use of a hydrological model to provide discharge at various points in the watershed allowed to overcome the lack of detailed measurements of discharge at locations other than the watershed outlet.

A REGIONALIZED RIVER WATER QUALITY MODEL CALIBRATION METHOD BASED ON WATERSHED PHYSICAL CHARACTERISTICS: APPLICATION TO THE CAU RIVER IN VIETNAM

Proposition d'une méthode de calage régionalisée pour les modèles de simulation de la qualité de l'eau en rivière : application à la rivière Cau au Vietnam

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ABSTRACT

A methodology is proposed for the calibration of river water quality models on large watersheds, in the absence of intensive measurements for water quality and quantity. This methodology is based on: 1) the use of the results from a hydrological model to provide the required hydrological variables to the water quality model; 2) five assumptions for the definition of initial and boundary conditions; 3) a three-step regionalized calibration method, in which the specific characteristics of the different subwatersheds are taken into account and 4) the adjustment of some parameters in order to reproduce processes that are not explicitly represented in the model. The regionalized calibration method relies on a comprehensive study of the land use and characteristics on each subwatershed and the definition of different sets of parameters values in distinct regions. Application to the Cau River, in Vietnam, with QUAL-GIBSI, an adaptation of the QUAL2E model, showed that: *i*) calibration and validation results were

significantly improved by applying regionalized calibration as compared to an initial calibration for which a single set of parameters values was used for the whole simulated river stretch and *ii*) use of a hydrological model to provide discharge at various points in the watershed allowed to overcome the lack of detailed measurements of discharge at locations other than the watershed outlet.

Key words: *QUAL2E, sensitivity analysis, parameter estimation, dissolved oxygen, phosphorus, nitrogen.*

RÉSUMÉ

Une méthodologie est proposée pour le calage de modèles de qualité de l'eau sur des bassins versants de grande taille où les mesures de qualité et de quantité d'eau sont rares. Cette

méthodologie est basée sur : 1) l'utilisation des résultats de simulation d'un modèle hydrologique pour fournir les valeurs de variables de nature hydrologique requises par le modèle de qualité de l'eau; 2) cinq hypothèses pour la définition des conditions initiales et aux limites; 3) une méthode de calage en trois étapes, prenant en compte les caractéristiques spécifiques des différents sous-bassins versants et 4) l'ajustement de la valeur de certains paramètres de façon à reproduire les processus qui ne sont pas explicitement représentés dans le modèle. La méthode de calage régionalisée se base sur une étude exhaustive de l'occupation du sol et des caractéristiques de chaque sous-bassin versant ainsi que sur la définition de différents jeux de valeurs de paramètres dans chaque région particulière. L'application de la méthode proposée sur la rivière Cau, au Vietnam, avec QUAL-GIBSI, une adaptation du modèle QUAL2E, a montré que : *i*) les résultats de calage et de validation sont améliorés grâce à la méthode de calage régionalisée par rapport à un calage initial, pour lequel un seul jeu de valeurs de paramètres a été utilisé pour tout le tronçon de rivière modélisé et *ii*) l'utilisation d'un modèle hydrologique pour fournir des valeurs de débits en différents points du bassin versant permet de surmonter le manque de données de débits mesurées ailleurs qu'à l'exutoire du bassin versant.

Mots-clés : *QUAL2E, analyse de sensibilité, estimation des paramètres, oxygène dissous, phosphore, azote.*

1. INTRODUCTION

River water quality models are useful in many contexts to predict or analyze the dynamic behaviour of rivers submitted to various external stressors, among which multiple point and nonpoint pollution sources, climate variability and so on. From the pioneer Streeter-Phelps model (STREETER and PHELPS, 1925) to more complex models including detailed description of biological processes related to sediment (e.g. RWQM1, REICHERT *et al.*, 2001), a multitude of river water quality models exist. From these models, the EPA QUAL2E model (BROWN and BARNWELL, 1987) would be the most widely used according to COX (2003) and KARADURMUS and BERBER (2004). Within the framework of integrated water resources management at the watershed scale, more specifically, river water quality models play an important role, mostly since they can provide assessments of the impact on water quality of various management options and/or intervention scenarios, before they are implemented in the field. To be used in such applications, river water quality models however require proper calibration and validation, based on sound observation data, for each watershed where they are meant to be applied. Calibration of river water quality models can be performed manually, by iteratively modifying the values of some parameters until a

satisfactory match is attained between simulated and observed values, or automatically, by optimizing one or more objective functions by using a numerical solver. Most applications of automatic calibration for river water quality models were performed on relatively small watersheds or river stretches. As for example, BERBER *et al.* (2009) calibrated the QUAL2E model on a 500 m stretch of the Yesilirmak River, Turkey, while YANG *et al.* (2000) calibrated the same model on a 9.3 km of the Ta-Chia River, Taiwan. When applied on larger areas, automatic calibration of river water quality models require intensive monitoring data, as for examples in CHO and HA (2010), for the QUAL2K model (CHAPRA *et al.*, 2007) on the Gangneung Namdaecheon River, South Korea, or in NG and PERERA (2003), for the QUAL2E model on the Yarra River, Australia.

Indeed, when simulating river water quality on a watershed covering many thousands square kilometers, it becomes difficult to finely adjust all parameters of the models when observation data are scarce. This is especially true since the value of many parameters can vary significantly through the watershed/river due to heterogeneous characteristics. In this case, manual calibration allows adapting the calibration strategy to the specific features of the river along its length. Lack of observation data and difficulties to acquire new data, required for the calibration of river water quality models, are particularly common in developing countries in South East Asia, Sub Saharan Africa, and Latin America. On one hand, this difficulty may be due to different factors, among which we find the lack of monetary or technical resources, and the lack of proper transportation facilities to reach strategic water quality monitoring locations. On the other hand, many existing river water quality problems in developing countries are expected to increase in the future due to the rapid demographic and economic growth (see HA *et al.*, 2017). Use of properly calibrated water quality models would therefore be more than useful to generate and test solutions to these problems at different spatial scales.

The first objective of this paper is to propose a methodology for proper calibration of river water quality models on large watersheds in the absence of intensive measurements for water quality and quantity. This methodology includes a regional calibration method to estimate the values of the model parameters and a method to define the model's boundary and initial conditions. This methodology is applied to the Cau River in Vietnam as a case study within the framework of an Integrated Watershed Management's project. The second objective is to show how hydrological modelling, at the watershed scale, can help to overcome the lack of monitoring data when calibrating river water quality models, since this situation is common in many developing countries.

2. METHODOLOGY

2.1 Study area

The Cau River watershed is located in Northern Vietnam and has a total area of 6 030 km² (Figure 1). The watershed covers the territory (either partially or entirely) of six Vietnamese provinces, which are Bac Kan, Thai Nguyen, Vinh Phuc, Ha Noi, Bac Ninh and Bac Giang. In this paper, we are studying only the part of the watershed located in the two upstream most provinces (Bac Kan and Thai Nguyen). This sub-watershed is illustrated in yellow color in figure 1. Elevation of the Cau River watershed varies from over 1 000 m in the Northern mountains to less than 100 m at the outlet. Generally, the slope direction of the watershed is from the North to the South and from the Northwest to the Southeast. The topography of the watershed includes three typical regions, mountains, valleys, and flat plains:

1. Mountains include the Tam Dao Range, on the western and southwestern side, and the Van On Range, on the northern and northeastern side. River Cau takes its source at Van On Mountain, at an elevation of 1 175 m. In this region, rivers are narrow with steep slopes on V shaped narrow valleys

enclosed between steep walls. This region is characterized by observations at the Thac Rieng station (Figure 2).

2. Valleys correspond to long valleys between mid-height hills. This region is the most populated in the watershed. Its rich silty soils are favorable to agriculture. This region is characterized by observations at the Thac Buoi station (Figure 2).

3. Plains are located at the most downstream part of the watershed, at an altitude of about 100 m. From Thai Nguyen City, capital of Thai Nguyen Province, to the watershed outlet, sediment deposits form large clay plains with sandy banks. This favors the intensification of agriculture and urban settlements. Various industrial activities are also present in this region. This region is characterized by observations at the Gia Bay station (Figure 2).

Mean annual temperature in the Cau River watershed varies around 23°C (DONRE BAC KAN, 2004 and DONRE THAI NGUYEN, 2004). Annual precipitation in the watershed varies from 1 500 mm to 2 700 mm. The rainfall season, which contributes from 85% to 90% of annual total precipitation, is from April to September (MoNRE, 1995). To illustrate the great variability of precipitation, which leads to

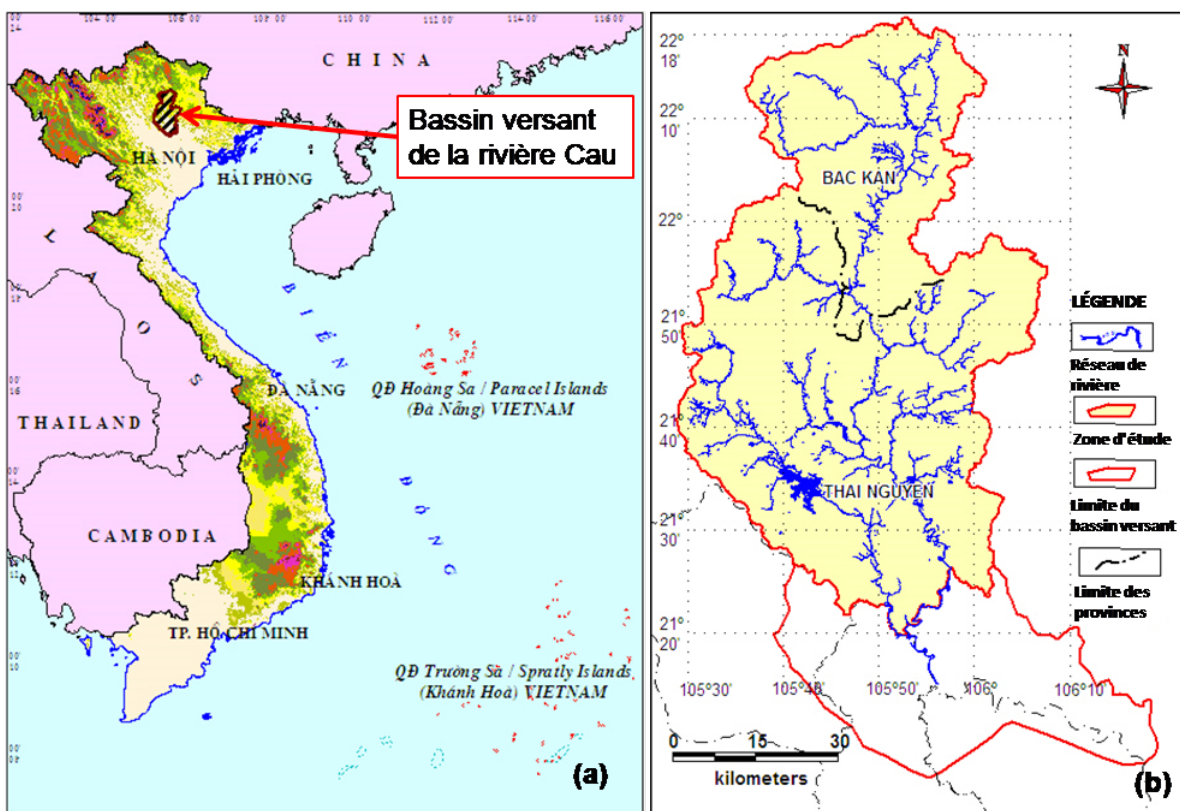


Figure 1. Location of the Cau River watershed.
Localisation du bassin versant de la rivière Cau.

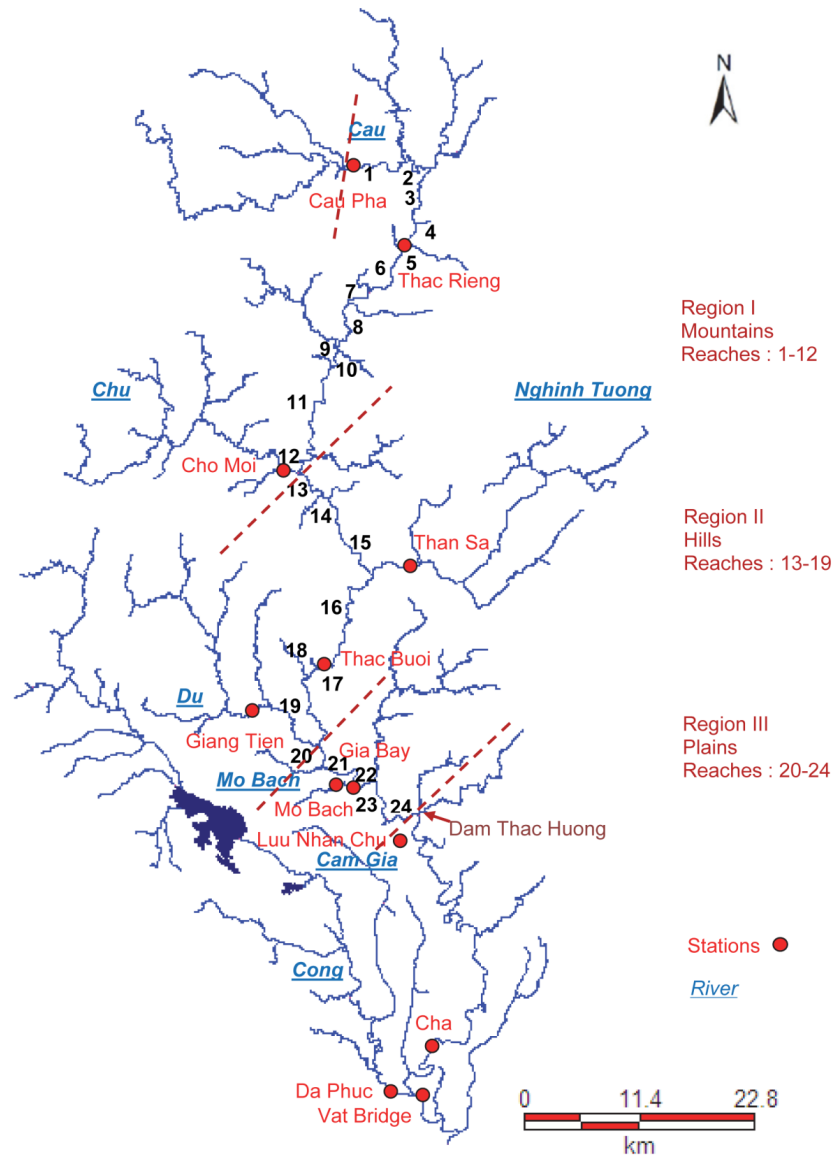


Figure 2 River network, monitoring stations, regions and simulation reaches.
Réseau de rivières, stations de mesures, régions et tronçons de simulation.

a great variability in river discharge, figure 3 shows the mean monthly discharge of Cau River at Gia Bay station (see figure 2 for its location) from 1997 to 2006.

Figure 4 shows the values of discharges measured during the four campaigns. Since water level and discharge are highly influenced by tides at Vat Bridge in the Cau River downstream of Gia Bay station (see figure 2 for its location), the water quality model was stopped at this station.

2.2 River water quality model

The mathematical model used to apply the proposed calibration strategy is an adaptation of the QUAL2E model (BROWN and BARNWELL, 1987), QUAL-GIBSI

(VILLENEUVE *et al.*, 1998). This model was chosen to model water quality for the Cau River, since the computer tool GIBSI (ROUSSEAU *et al.*, 2000) is currently applied on this watershed, in the frame of an integrated water management project. GIBSI is a computer tool designed to assist decision makers in their assessment of various river basin management scenarios in terms of typical water physical and chemical parameters and standards for various uses of the water (ROUSSEAU *et al.*, 2000). It includes simulation models (hydrology, soil erosion, agricultural-chemical transport, and water quality) and management modules. These modules are used to build scenarios by modifying either pollution sources, agricultural practices or some watershed characteristics (e.g. land use). The impact of these scenarios on water quality and quantity can then be assessed by applying the simulation models. QUAL-GIBSI was adapted from QUAL2E in order

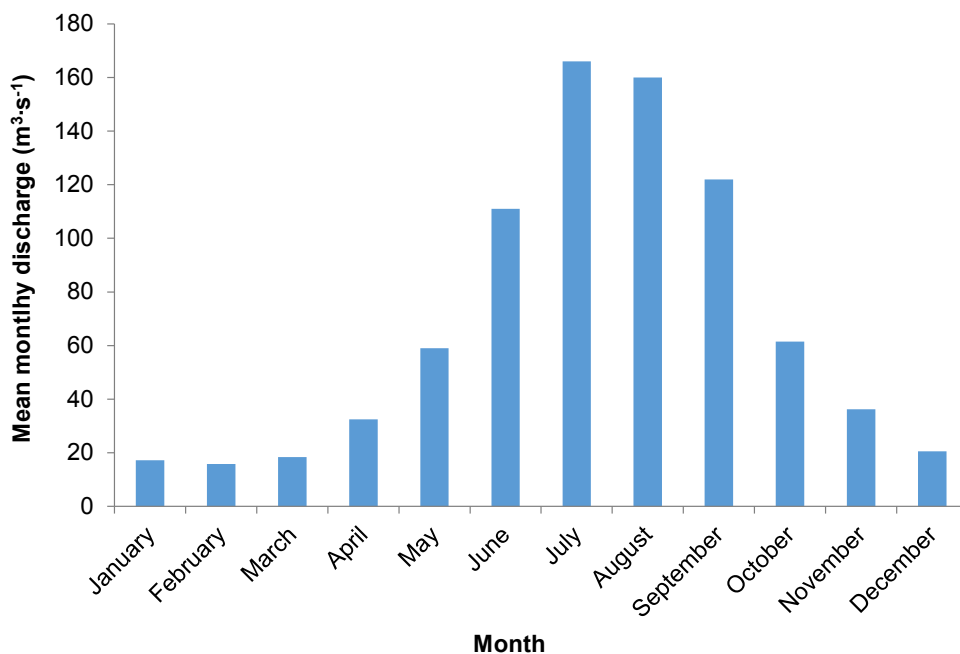


Figure 3. Mean monthly discharge at the Gia Bay station, from 1997 to 2006.
Débit mensuel moyen à la station Gia Bay, de 1997 à 2006.

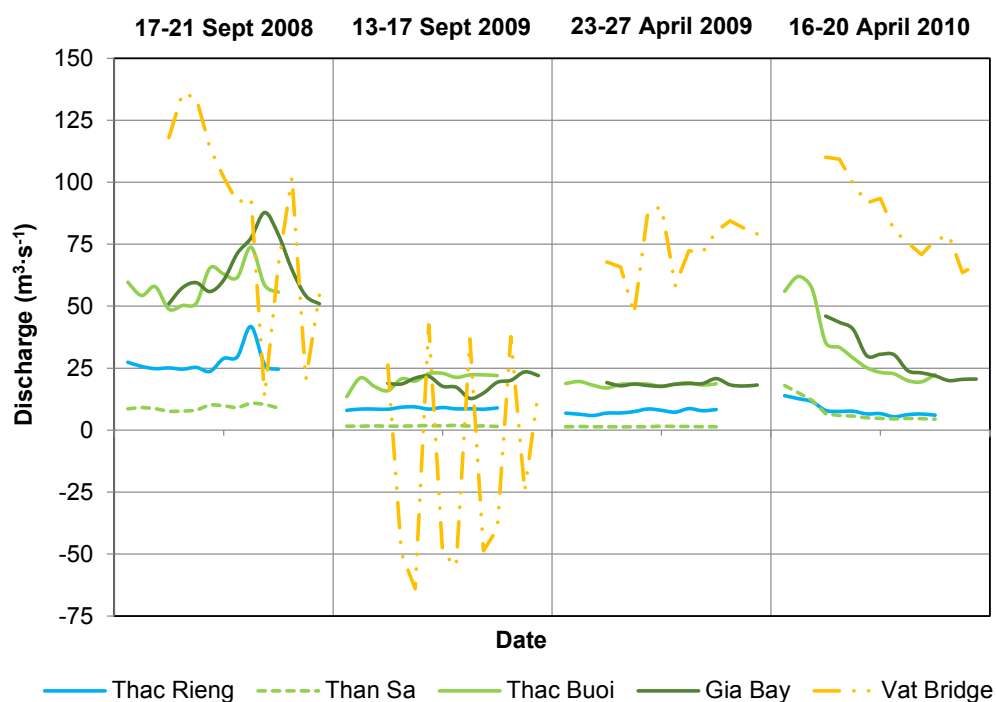


Figure 4. Discharge during the four campaigns, three times per day.
Débit pendant les quatre campagnes de mesures, trois fois par jour.

to be compatible with the other simulation models in GIBSI and also to fulfill the requirements of integrated watershed management. The adaptations were to: 1) increase the maximal number of river reaches; 2) use the water flow variables (velocity, discharge, water height) simulated by the hydrological Hydrotel model (FORTIN *et al.*, 2001), included in GIBSI; 3) add a dilution term in the advection-dispersion equation to allow the simulation of successive permanent states with varying discharge values (simulated with the Hydrotel model); 4) read new data concerning diffuse and point pollution sources at each time step; 5) modify the heat exchange module in order to take into account the exchanges between water and the river bed; 6) add the ROTO model (ARNOLD *et al.*, 1995) to simulate stream deposition, bed erosion and sediment transport; 7) add the maximal number of non-conservative substances. Details concerning the equations of QUAL2E and QUAL-GIBSI can be found in BROWN and BARNWELL (1987) and VILLENEUVE *et al.* (1998) respectively.

2.3 Water quality data

Four river water monitoring campaigns were carried out on the Cau River watershed in September 2008, January 2009, April 2009 and April 2010 by the Vietnamese Academy of Science and Technology (VAST). Location of the stations where samples were collected is shown on figure 2. During these

campaigns, discharge, temperature, pH, and concentration in suspended solids, dissolved oxygen (DO), five-day biochemical oxygen demand (BOD₅), coliforms, chlorophyll *a*, organic nitrogen, ammonia (N-NH₄), nitrites, nitrates, organic phosphorus and dissolved phosphorus were measured. Details about the applied analytical methods are given in VAST (2008, 2009a, 2009b and 2010).

For each of the four campaigns, three measurements per day (8:00, 12:00 and 16:00) were realized during four days, for each constituent, at Than Sa station, on Nghinh Tuong River, and at three stations on the Cau River (Thac Rieng, Thac Bui and Gia Bay). Samples were also taken once a day during five days on three tributaries of the Cau River (Chu, Du and Cong Rivers) and in a municipal (Mo Bach) and industrial (Luu Nan Chu) discharge. Table 1 summarizes the location and number of measurements for each campaign.

All these data were illustrated graphically to evaluate correspondences and interrelations between nutrients. For examples, figure 5 shows the repartition of the values of dissolved oxygen, suspended sediments and organic phosphorus for all the campaigns and figure 6 illustrates the values measured during the first campaign, in September 2008, when the discharges were high, around 60 m³.s⁻¹ near Thac Bui and Gia Bay stations.

Table 1. Details of the monitoring campaigns.
Tableau 1. Détails des campagnes de mesures.

River or discharge	Station	September 2008	January 2009	April 2009	April 2010
Nghinh Tuong	Than Sa	3 times/day from 17 to 20	3 times/day from 13 to 16	3 times/day from 23 to 26	3 times/day from 16 to 19
Cau	Thac Rieng	3 times/day from 17 to 20	3 times/day from 13 to 16	3 times/day from 23 to 26	3 times/day from 16 to 19
Cau	Thac Bui	3 times/day from 17 to 20	3 times/day from 13 to 16	3 times/day from 23 to 26	3 times/day from 16 to 19
Cau	Gia Bay	3 times/day from 18 to 21	3 times/day from 14 to 17	3 times/day from 24 to 27	3 times/day from 17 to 20
Cau	Cha	–	3 times/day from 14 to 17	3 times/day from 24 to 27	3 times/day from 17 to 20
Cau	Vat Bridge	3 times/day from 18 to 21	3 times/day from 14 to 17	3 times/day from 24 to 27	3 times/day from 17 to 20
Chu	Cho Moi	1 time/day from 17 to 21	1 time/day from 13 to 17	1 time/day from 23 to 27	1 time/day from 16 to 20
Du	Giang Tien	1 time/day from 17 to 21	1 time/day from 13 to 17	1 time/day from 23 to 27	1 time/day from 16 to 20
Municipal discharge	Mo Bach	1 time/day from 17 to 21	1 time/day from 13 to 17	1 time/day from 23 to 27	1 time/day from 16 to 20
Industrial discharge	Luu Nhan Chu	1 time/day from 17 to 21	1 time/day from 13 to 17	1 time/day from 23 to 27	1 time/day from 16 to 20
Cong	Da Phuc	1 time/day from 17 to 21	1 time/day from 13 to 17	1 time/day from 23 to 27	1 time/day from 16 to 20

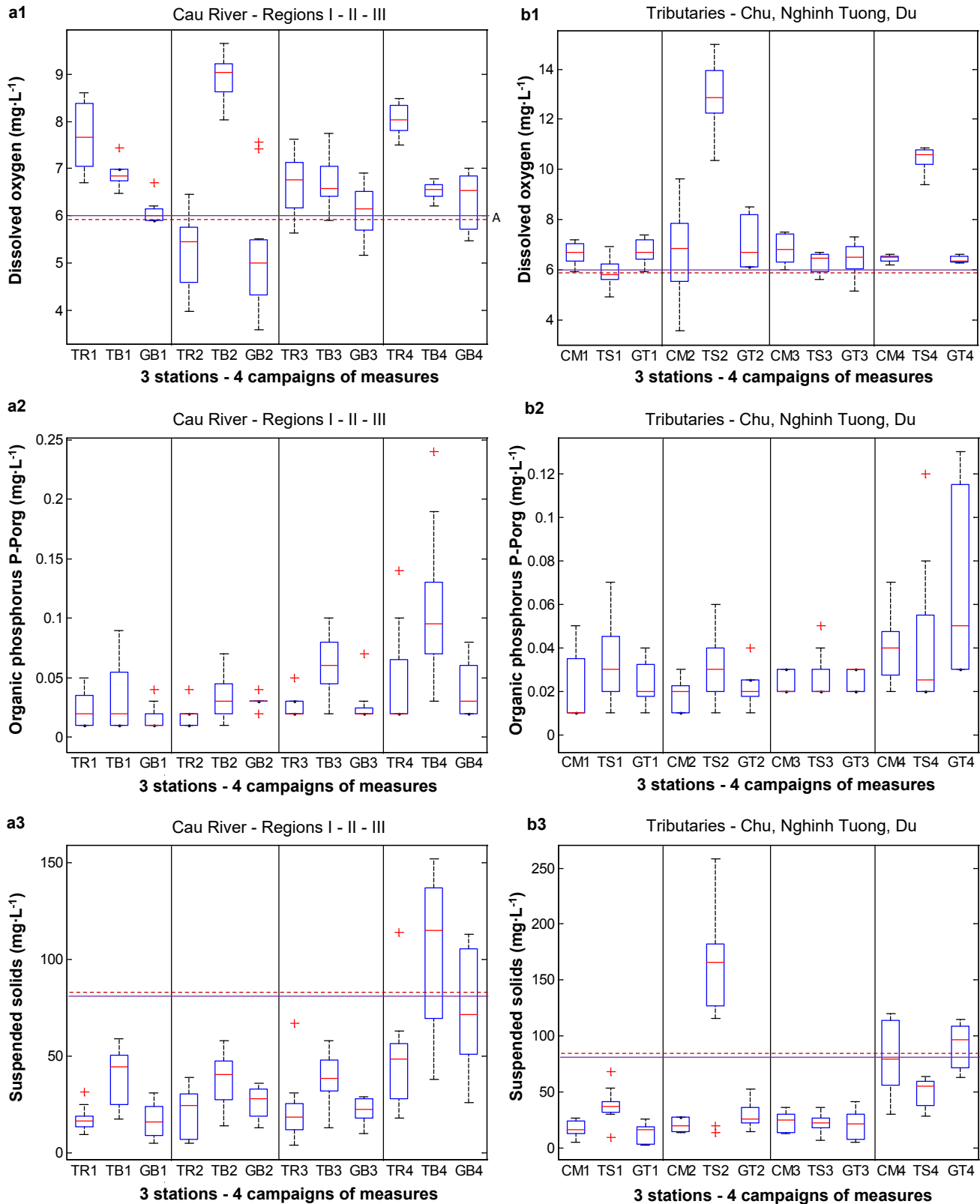


Figure 5. Observed concentrations of dissolved oxygen (a1-b1), organic phosphorus (a2-b2) and suspended solids (a3-b3). Letters represent the station: a) Cau River: Thac Rieng (TR), Thac Buoi (TB), Gia Bay (GB); b) Tributaries: Cho Moi (CM), Than Sa (TS), Giang Tien (GT). Numbers represent the campaigns: 1 (Sept 2008), 2 (Jan 2009), 3 (April 2009), 4 (April 2010). The horizontal lines represent the Vietnamese standards: A) for dissolved oxygen for water supply (≥ 6 mg·L⁻¹) and B) for suspended solids for agriculture (< 80 mg·L⁻¹).

Concentrations mesurées en oxygène dissous (a1-b1), phosphore organique (a2-b2) et matières en suspension (a3-b3). Les lettres représentent la station: a) rivière Cau : Thac Rieng (TR), Thac Buoi (TB), Gia Bay (GB); b) affluents : Cho Moi (CM), Than Sa (TS), Giang Tien (GT). Les nombres représentent la campagne de mesures: 1 (sept. 2008), 2 (janv. 2009), 3 (avril 2009), 4 (avril 2010). Les lignes horizontales représentent les critères vietnamiens pour : A) l'oxygène dissous pour l'alimentation en eau (≥ 6 mg·L⁻¹) et B) les matières en suspension pour les usages agricoles (< 80 mg·L⁻¹).

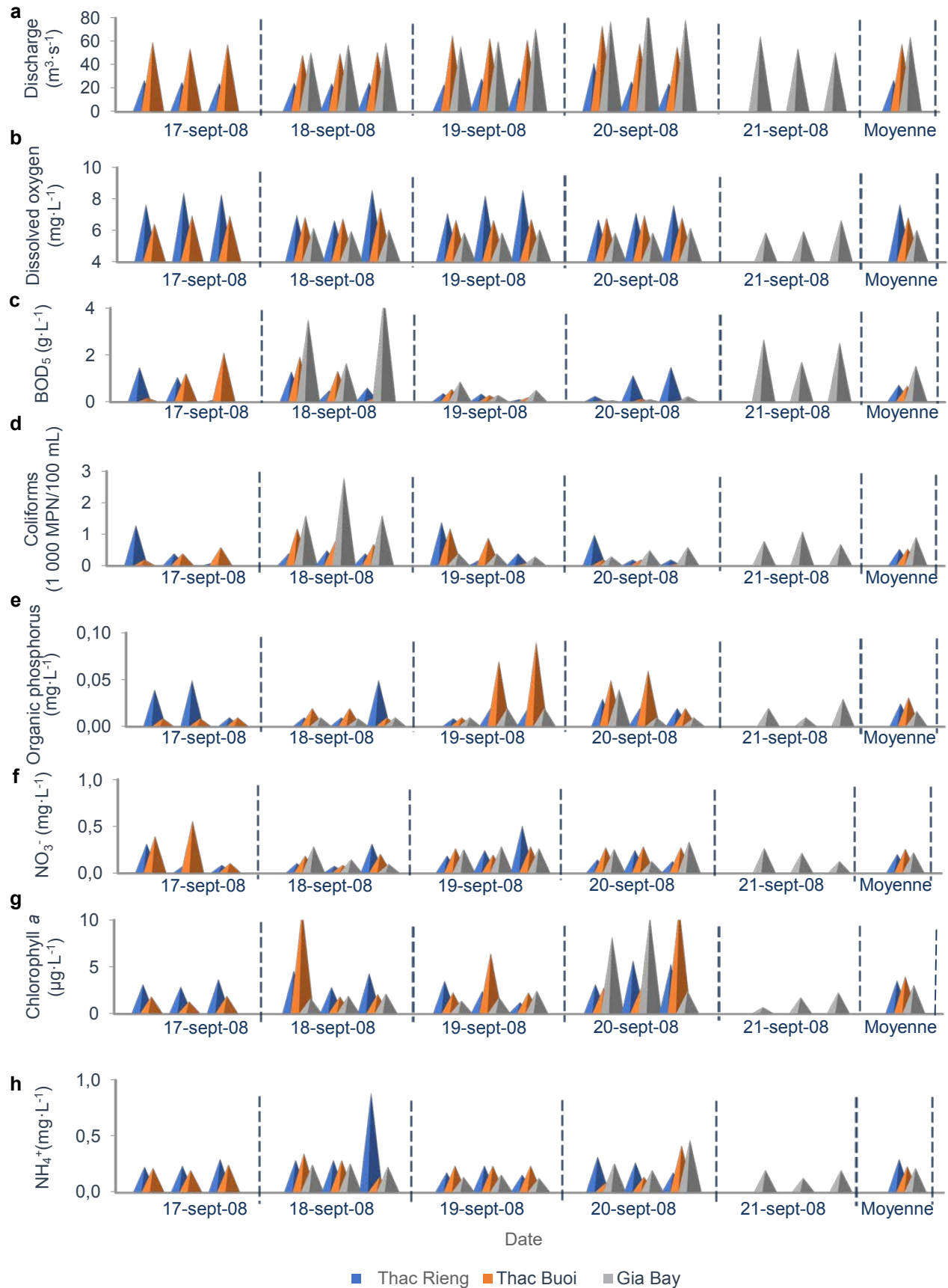


Figure 6. Measures from 17 to 21 September 2008 (8:00, 12:00, 16:00): a) discharge, b) dissolved oxygen, c) BOD_5 , d) coliforms, e) organic phosphorus, f) NO_3^- , g) chlorophyll *a*, and h) NH_4^+ .
 Mesures du 17 au 21 septembre 2008 (8:00, 12:00, 16:00) : a) débit, b) oxygène dissous, c) DBO_5 , d) coliformes, e) phosphore organique, f) NO_3^- , g) chlorophylle *a* et h) NH_4^+ .

2.4 Model implementation

Only the Cau River was included in the QUAL-GIBSI model for this application; the tributaries of the Cau River were considered as point loads in the model. The river was divided in 24 reaches, for a total of 125 km river length, as illustrated in figure 2. Water quality was simulated for 12 different days (18, 19 and 20 September 2008; 14, 15 and 16 January 2009; 24, 25 and 26 April 2009; 17, 18 and 19 April 2010). For each simulation day, river discharge must be given as input to the QUAL-GIBSI model, for each of the 24 river reaches. Since river discharge was measured at only a few monitoring stations during the monitoring campaigns, river discharges simulated by the Hydrotel model (FORTIN *et al.*, 2001; calibrated for the Cau River watershed by NGUYEN (2012) were used as input for the 24 river reaches. Initial and limit conditions were determined based on five main assumptions listed below.

Assumption 1 concerns the spatial transposition of initial concentrations. For reaches where the concentration of water quality constituents was measured three times per day, their daily means were applied as initial conditions. For reaches where no measurement was taken, the initial concentrations were set to the mean values measured at the stations located in the same region, where regions are defined as detailed in section 2.5. Assumption 2 concerns the weighting of initial concentrations at the confluence with important tributaries. For reaches located at the confluence with the Chu River, the Nghinh Tuong River and the Du River, the initial concentrations were estimated as the mean weighted value between concentrations in the tributary and in the Cau River, where the weights corresponded to the mean discharge in each river. Assumption 3 relates to the spatial transposition of loads coming from ungaged tributaries. Hydrological variables (discharge, water level and velocity) for the 23 tributaries included in the model were simulated with the Hydrotel model. For water quality however, concentrations are measured on only three tributaries (Chu, Nghinh Tuong and Du rivers). For the other 20 tributaries, the initial conditions for concentrations were set to the mean values measured in the gaged tributary located in the same region, where regions are defined as detailed in section 2.5. Assumption 4 deals with the computation of diffuse discharge along the river reaches. Those were computed from the Hydrotel model's results, as the difference, for each reach, between the upstream and downstream discharge (from which, when applicable, the discharge of the tributary on this reach was subtracted). Finally, assumption 5 relates to diffuse loads. For these loads, concentrations were assumed to be equal to the mean daily observed concentrations in the Cau River.

2.5 Calibration and validation method

The applied calibration method consists of three main steps which are: 1) initial calibration; 2) sensitivity analysis; and 3) regional calibration. The simulated water variables are DO, BOD₅, coliforms, chlorophyll *a*, organic nitrogen, N-NH₄, nitrites, nitrates, organic phosphorus and dissolved phosphorus. The initial calibration was undertaken to provide parameter values to be used for sensitivity analysis. For both initial calibration and sensitivity analysis, parameters of the QUAL-GIBSI model were kept constant for all of the river reaches, while they varied between regions for the regional (final) calibration.

Three efficiency criteria were used to quantify the model performance for each day simulated during calibration and validation:

1. An objective function, $Obj_{v,i}$, that quantifies the relative difference between the observed and simulated values for each simulated water quality variable at each monitoring station, computed with:

$$Obj_{v,i} = 100 \left(\frac{C_{s_{v,i}} - C_{m_{v,i}}}{C_{m_{v,i}}} \right) \quad (1)$$

where $i = 1, 2, \text{ or } 3$ respectively for the Thac Rieng, Thac Bui and Gia Bay monitoring stations; $C_{s_{v,i}}$ = mean simulated value per day and $C_{m_{v,i}}$ = mean measured value per day for 3 days of a monitoring campaign at station i for water quality variable v ;

2. An objective function, Obj_v , that quantifies the relative difference between the observed and simulated values, averaged in absolute value over all 3 monitoring stations for each simulated water quality variable, computed with:

$$Obj_v = \frac{\sum_{i=1}^n \left| 100 \left(\frac{C_{s_{v,i}} - C_{m_{v,i}}}{C_{m_{v,i}}} \right) \right|}{n} \quad (2)$$

where $n = 3$, number of monitoring station for a water quality variable v ;

3. An objective function, Obj , that quantifies the overall performance per day of the model for the 3 monitoring station and the 10 simulated water quality variables, computed with:

$$Obj = \frac{\sum_{v=1}^T \sum_{i=1}^n \left| 100 \left(\frac{C_{s_{v,i}} - C_{m_{v,i}}}{C_{m_{v,i}}} \right) \right|}{T} \quad (3)$$

where $T = 10$, number of simulated water quality variables.

Finally, the results were compiled for three days during each campaign and their mean and standard deviation were calculated. Only the mean results for the two last criteria will be presented in this paper. One should note that a total of 270 measured data were used for the calibration process (3 stations * 3 monitoring campaigns * 3 days per campaign * 10 measured variables). Indeed, the ten water quality variables that are simulated are all connected in the equations of the model, so calibration cannot be performed in a sequential manner for each of the ten variables.

Initial calibration was based on the simulations and observations for September 2008, January 2009 and April 2009 monitoring campaigns. Some values of the parameters listed in table 2 were varied manually from their default values (taken from BROWN and BARNWELL, 1987) or from their mean value when a range is suggested in BROWN and BARNWELL (1987). All kinds of settling and decay rates, except BOD and nitrite decay rates (K_1 , β_3), were set to zero during the initial calibration to minimize the impact of sedimentation; these parameters were adjusted further during the regional calibration. For F (fraction of algal nitrogen uptake from ammonium pool), initial value was set to 0.5 instead of 0.9. For the initial calibration, the O'CONNOR and DOBBINS (1958) equation was used to compute the reaeration rate K_2 (option 3 in QUAL2E). The calibration was stopped when a better value of Obj could not be achieved.

Sensitivity analysis was performed by varying the parameter values by $\pm 50\%$ around a "mean" value which was either: 1) the value issued from initial calibration, for the parameters for which this value is different than zero (μ , ρ , α_0 , F); 2) for the parameters for which the value issued from initial calibration was equal to zero and for which BROWN and BARNWELL (1987) propose a range in the positive numbers domain, either the central value of this range (for σ_1 , σ_4 and σ_5) or a value chosen in such a way that all the parameter values used during the sensitivity analysis remained in this range (for K_1 , K_5 , β_1 , β_2 , β_3 and β_4); and 3) for the parameters for which the value issued from initial calibration was equal to zero and for which BROWN and BARNWELL (1987) propose a default value equal to zero (K_4 , σ_2 and σ_3), a value chosen to get a range of variation similar to those of the parameters representing similar processes. For the only parameter for which the range proposed by BROWN and BARNWELL (1987) covers negative and positive values (K_3), only positive values were considered during sensitivity analysis. Finally, option 1 (values entered by the user) was used for the reaeration rate (K_2) because it is the only option that allows manual variation of K_2 . Since the range of values proposed by BROWN and BARNWELL (1987) for K_2 led to simulated DO values that were too far from the observed value, a mean value of 2 d^{-1} was used instead.

The relative variation of each water quality state variable was computed as a function of each of the 18 parameters listed in table 2 as follows:

$$\Delta_{v,\theta} = \frac{\frac{Cs_{v+} - Cs_{v-}}{Cs_v}}{\frac{\theta_{+50\%} - \theta_{-50\%}}{\theta_m}} = \frac{Cs_{v+} - Cs_{v-}}{Cs_v} \quad (4)$$

where $\Delta_{v,\theta}$ = relative variation of water quality variable v as a function parameter θ ; Cs_{v+} = simulated value of water quality variable v with θ increased by 50% (all other parameters keeping their mean values); Cs_{v-} = simulated value of water quality variable v with θ decreased by 50% (all other parameters keeping their mean values); Cs_v = simulated value of water quality variable v with mean values for all parameters; $\theta_{+50\%}$ = mean value of parameter θ increased by 50%; $\theta_{-50\%}$ = mean value of parameter θ decreased by 50%; θ_m = mean value of parameter θ .

Results of the sensitivity analysis provided guidance for the final step of calibration, the regional calibration. This means that the parameters to which the results of the models were shown to be the most sensitive were those that were first varied during the calibration process. During this final calibration, three different set of parameters' values were defined. Once again, the calibration was performed based on the Obj value (see equation 3) and was stopped when a better value for Obj could not be achieved. Each of the three sets of parameters was used in a specific region. Regions were delimited based on topography and land use. The three monitoring stations are representative of each region, since they reflect the diversity in land use and topography encountered throughout the watershed. The three regions are identified as I, II and III in figure 2 and their main characteristics are given in table 3.

As for the initial calibration, the regional calibration was based on the simulations and observations for the September 2008, January 2009 and April 2009 monitoring campaigns (Figures 5 and 6). Finally, validation of the calibrated model was performed based on the simulations and observations for April 2010 monitoring campaigns, with simulated values obtained using the parameters' values issued from the regional calibration.

For the regional calibration and the validation, the reaeration rate, K_2 , was computed using the equation developed by CHURCHILL *et al.* (1962) (option 2 in QUAL2E). Indeed, it was found that this equation allowed a better representation of the spatial variations in DO concentration. Consequently, for initial calibration, the value of 17 parameters had to be estimated, while for regional calibration, 51 parameter values (17 parameters * 3 stations) were estimated.

Table 2. Values of the parameters for the initial and regional calibrations.
Tableau 2. Valeurs des paramètres pour les calages initial et régional.

Parameter (rate)	Unit	Initial calibration	Regional calibration		
			I	II	III
			Mounts	Hills	Plains
α_0 Ratio of chlorophyll <i>a</i> to algal biomass	%	10%	10%	10%	10%
μ Algal growth	d ⁻¹	2.2	1.2	1.2	1.2
ρ Algal respiration	d ⁻¹	0.12	0.12	0.12	0.12
<i>F</i> Fraction of algal N uptake from ammonium pool	–	0.5	0.5	0.5	0.5
β_1 Ammonium decay → N-NO ₂	d ⁻¹	0	0	0	0.06
β_2 Nitrite decay → N-NO ₃	d ⁻¹	0	0	0	2
β_3 Organic N decay → N-NH ₄	d ⁻¹	0.02	0.02	0.02	0
β_4 Organic P decay → dissolved P	d ⁻¹	0	0.01	0.02	0
K_1 BOD decay	d ⁻¹	0.02	0.2	0.2	0.2
K_2 Reaeration	d ⁻¹	Opt. 3	Opt. 2	Opt. 2	Opt. 2
K_3 BOD settling	d ⁻¹	0	-0.025	0.25	-0.25
K_4 SOD uptake	mg O·m ⁻² ·d ⁻¹	0	0.5	1	6
K_5 Coliform decay	d ⁻¹	0	0	0.05	-0.2
σ_1 Algal settling	m·d ⁻¹	0	0.6	0.9	1.2
σ_2 Benthic dissolved P source	mg P·m ⁻² ·d ⁻¹	0	0	2.00	-2.00
σ_3 Benthic ammonium source	mg N·m ⁻² ·d ⁻¹	0	-0.10	-0.50	-1.00
σ_4 Organic N settling	d ⁻¹	0	0.001	0.001	0.1
σ_5 Organic P settling	d ⁻¹	0	0	-0.05	1

Table 3. Characteristics of the three regions for the regional calibration.
Tableau 3. Caractéristiques des trois régions pour le calage régionalisé.

Region	Station	Main land use	Regionalization criterion
Mountains	Thac Rieng	Forest	≤40% agriculture, ≤10% urban
Valleys	Thac Buoi	Agriculture	≥40% agriculture, ≤10% urban
Plains	Gia Bay	Urban areas	≥10% urban

3. RESULTS AND DISCUSSION

3.1 Sensitivity analysis

The value of $\Delta_{v,\theta}$ was computed for all possible combinations of the ten water quality variables (*v*) and 18 calibration parameter (θ), for a total of 180 evaluations. Table 4 presents a summary of the sensitivity analysis results, where only the greatest $\Delta_{v,\theta}$ values are shown for each water quality variable *v*. In table 4, some parameters can appear more than once, if they have a significant influence on more than one water quality variable (for example β_1 , which has a significant impact on ammonium and on nitrites). From table 4, it can be seen that the parameters to which the results of the model are the most sensitive are:

- for nitrites: β_1 (68.2%) and β_2 (-25.1%);
- for chlorophyll *a*: μ (40.1%) and σ_1 (-36.6%);

- for ammonium: β_1 (-13.3%);
- for BOD₅: K_3 (-10.3%);
- for DO: K_2 (8.5%).

Calibration of the model should then focus primarily on these parameters, depending on the water quality variable that needs to be better simulated.

In previous studies, it was found by YANG *et al.* (2000) and KIM and JE (2006), both studies conducted on Asian rivers, that the concentration of chlorophyll *a* was most sensitive to the algal maximum growth rate (μ) and algal respiration rate (ρ). In our case, the simulated concentration of chlorophyll *a* is most sensitive to the algal settling rate (σ_1 ; -36.6%) than to ρ (-7.6%). This could be due to differences in the ranges of values selected for the sensitivity analysis. Concerning the simulated concentration of DO, it proves to be most sensitive to the BOD decay rate (K_1) in KIM and JE (2006) and to the reaeration rate (K_2) in YANG *et al.* (2011; also in Asia). For the Cau River, the simulated concentration of DO is also most sensitive to K_2 . However the observed and simulated concentrations in BOD were higher in KIM and JE (2006; Anyang River in Korea) than in the two other studies (YANG *et al.* [2011] and this one), explaining why the BOD decay rate had a higher influence than the reaeration rate on the concentration of DO in KIM and JE (2006).

Table 4. Data and results of the sensitivity analysis.
Tableau 4. Données et résultats de l'analyse de sensibilité.

State variable	Parameter (rate)	Unit	Minimum value	Mean value	Maximum value	$\Delta_{v,2}$ (%)
DO	K_2 Reaeration	d^{-1}	1	2	3	8.5
	K_4 SOD uptake	$mg\ O \cdot m^{-2} \cdot d^{-1}$	1	2	3	-3.4
BOD ₅	K_3 BOD settling	d^{-1}	0.1	0.2	0.3	-10.3
	K_7 BOD decay	d^{-1}	0.02	0.04	0.06	-2.3
Coliforms	K_5 Coliform decay	d^{-1}	0.05	0.1	0.15	-5.8
Chlorophyll <i>a</i>	μ Algal growth	d^{-1}	1.1	2.2	3.3	40.1
	σ_1 Algal settling	$m \cdot d^{-1}$	1	2	3	-36.6
	ρ Algal respiration	d^{-1}	0.06	0.12	0.18	-7.6
	α_0 Ratio of chlorophyll <i>a</i> to algal biomass	%	5%	10%	15%	0.8
Organic N	σ_4 Organic N settling	d^{-1}	0.025	0.05	0.075	-2.6
	β_3 Organic N decay \rightarrow N-NH ₄	d^{-1}	0.02	0.04	0.06	-2.3
Ammonium	β_3 Organic N decay \rightarrow N-NH ₄	d^{-1}	0.02	0.04	0.06	3.3
N-NH ₄	β_1 Ammonium decay \rightarrow N-NO ₂	d^{-1}	0.1	0.2	0.3	-13.3
	σ_3 Benthic ammonium source	$mg\ N \cdot m^{-2} \cdot d^{-1}$	0.025	0.05	0.075	0.01
Nitrites	β_1 Ammonium decay \rightarrow N-NO ₂	d^{-1}	0.1	0.2	0.3	68.2
N-NO ₂	β_2 Nitrite decay \rightarrow N-NO ₃	d^{-1}	0.2	0.4	0.6	-25.1
Nitrates	β_2 Nitrite decay \rightarrow N-NO ₃	d^{-1}	0.2	0.4	0.6	1.0
N-NO ₃	F Fraction of algal nitrogen uptake from ammonium pool	-	0.25	0.5	0.75	1.0
	N-NH ₄ / (N-NH ₄ + N-NO ₃)					
Organic P	σ_5 Organic P settling	d^{-1}	0.025	0.05	0.075	-2.7
	β_4 Organic P decay \rightarrow dissolved P	d^{-1}	0.01	0.02	0.03	-1.2
Dissolved P	β_4 Organic P decay \rightarrow dissolved P	d^{-1}	0.01	0.02	0.03	2.8
	σ_2 Benthic dissolved P source	$mg\ P \cdot m^{-2} \cdot d^{-1}$	0.025	0.05	0.075	1.1

3.2 Calibration and validation

Table 2 presented before gives the values of the parameters issued from the initial and regional calibrations, while table 5 presents the results of both calibrations as well as of validation. As mentioned before, the state variables were simulated for nine different days during both calibrations (18, 19 and 20 September 2008; 14, 15 and 16 January 2009; 24, 25 and 26 April 2009) and for three days during validation (17, 18 and 19 April 2010). The values in table 5 are the mean values of the objective function averaged over these days and over the three monitoring stations, while the errors presented (following the symbol “ \pm ”) are the standard deviations between these values. Good values are those for which both the mean value of *Obj* (or *Obj_v*) and its standard deviation are low. Figures 7 and 8 show some simulation results for chlorophyll *a*, N-NO₂, organic P and dissolved P. Complete results for all simulated state variables are given in AUDET (2013).

Results in table 5 (as well as in figures 7 and 8) show that the calibration results are significantly improved by applying regionalization as compared to the initial calibration for all simulated state variables, except for BOD₅ and coliforms for which the calibration are similar between the initial and regional

Table 5. Calibration and validation results.
Tableau 5. Résultats de calage et de validation.

State variable	Initial calibration	Regional calibration	Validation
Objective value averaged over the three monitoring stations (<i>Obj_v</i>)			
DO	11 \pm 7	7 \pm 5	9 \pm 2
BOD ₅	12 \pm 12	14 \pm 8	13 \pm 2
Coliforms	21 \pm 15	21 \pm 14	39 \pm 27
Chlorophyll <i>a</i>	49 \pm 27	15 \pm 11	9 \pm 4
Organic N	8 \pm 5	7 \pm 4	6 \pm 1
Ammonium	12 \pm 7	11 \pm 6	13 \pm 2
N-NH ₄			
Nitrites N-NO ₂	86 \pm 245	27 \pm 58	16 \pm 4
Nitrates N-NO ₃	6 \pm 3	5 \pm 3	9 \pm 2
Organic P	23 \pm 18	9 \pm 8	10 \pm 1
Dissolved P	19 \pm 12	10 \pm 8	5 \pm 0
Mean objective averaged over the three monitoring stations (<i>Obj</i>)			
	25 \pm 25	13 \pm 6	13 \pm 2

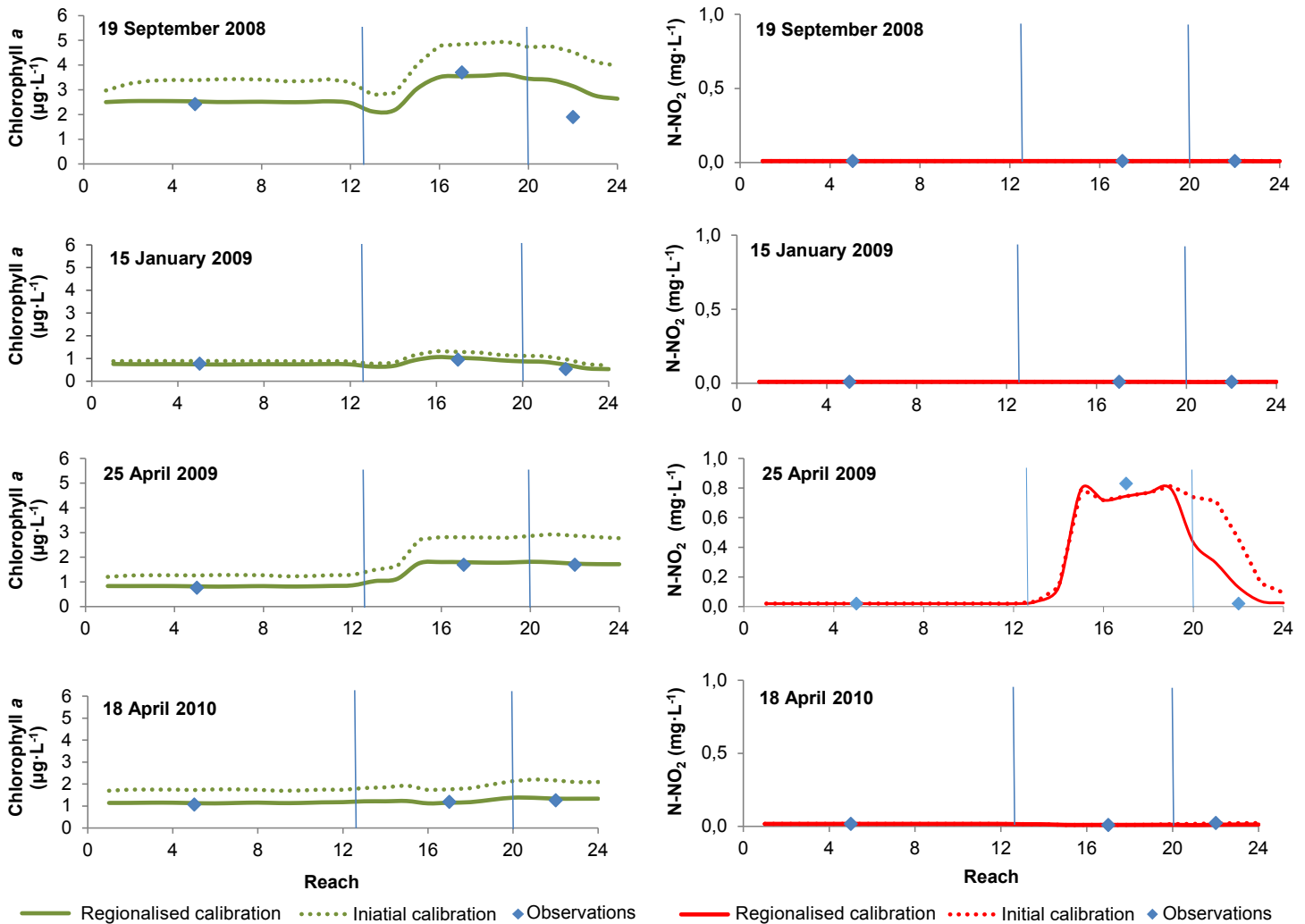


Figure 7. Examples of simulation results for chlorophyll *a* and N-NO₂.
Exemples de résultats de simulation pour la chlorophylle a et le N-NO₂.

calibrations. Overall, the mean objective function (averaged over all state variables) is significantly better in regional than in initial calibration. Use of the parameters obtained from the regional calibration also leads to good results during the validation period. Improvements of the results from the initial to the regional calibration are mainly due to the variation of the parameters between the three regions, which allows taking into account the differences between the regions in terms of topography and land use.

The variations of the parameter values among the three regions, in the regional calibration, are dictated by differences in land use and physiographic characteristics. For each region, some parameters can also be adjusted in order to reproduce processes that are not explicitly modeled in QUAL2E. As for example, the concentration of coliforms in QUAL2E is modeled as a simple first order decay reaction, without any interaction with the other water quality variables. However, it is well known that high concentrations of coliforms can lead to

reductions in dissolved oxygen concentrations (see for example DAVIES-COLLEY *et al.*, 1999, or figure 6). To take this into account, variations in the value of K_4 , the sediment oxygen demand (SOD) uptake rate, can represent real variations in SOD, but also the variations of oxygen demand for the degradation of coliforms, or for any other oxygen demanding process. This is why the value of K_4 for the final calibration is higher in Region III than in the two other regions, to reproduce the oxygen demand from coliforms in this urbanized area.

All other calibration parameters can be similarly adjusted as a function of land use and topographical characteristics in each region. Thus σ_1 , the algal settling rate, was given increasing values from Region I to Region III, due to decreasing water velocity (decreasing river slopes) from upstream to downstream. For the same reason, coliforms travel rapidly in Region I, leading to rapid variations in coliforms concentrations in this area. The variation of these concentrations in Region I can thus be modeled based only on water transport, without taking

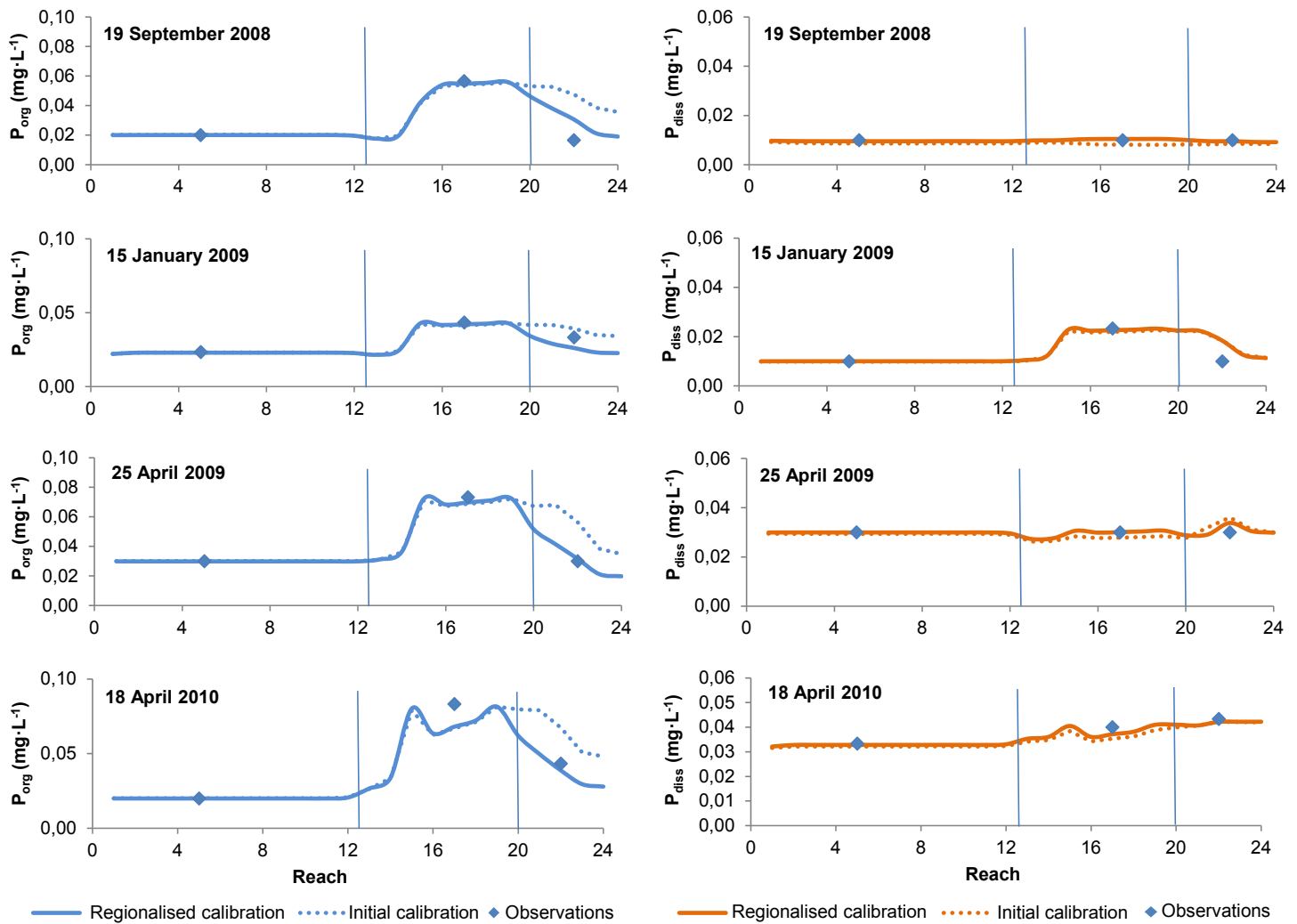


Figure 8. Examples of simulation results for organic and dissolved phosphorus.
Exemples de résultats de simulation pour le phosphore organique et dissous.

into account a mortality rate (hence a value of 0 d^{-1} for K_5 , the coliform decay rate, in Region I). In Region II, water velocities are lower and a decay rate is required to reproduce the self-purification capacity of the river ($K_5 = 0.05 \text{ d}^{-1}$). In Region III, massive coliform inputs are brought by the Du River and by untreated municipal wastewater discharges. These inputs most often exceed the self-purification capacity of the river, hence a negative rate of -0.2 d^{-1} for K_5 in the urbanized region (Region III).

As for dissolved phosphorus, the benthic source was set to $0 \text{ mg P} \cdot \text{m}^{-2} \text{ d}^{-1}$ in Region I, due to the low sedimentation rate in the mountainous area, while in Region II, mostly agricultural, the bio-dynamism could foster a higher P contribution from benthos ($\sigma_2 = 2 \text{ mg P} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$). In Region III, benthos is largely affected by industrial and municipal wastewater discharges, which could lead to decrease in the benthic contribution to dissolved phosphorus. Moreover, the high dissolved P contribution from untreated wastewater discharges in this

region combined with low river flow velocities cause a net loss from dissolved P from the water column to the sediments, hence a negative value for σ_2 in Region III ($-2 \text{ mg P} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$).

Concerning σ_5 , the settling rate of organic P, it was set to 0 d^{-1} in the upstream region since sedimentation is very low, if not absent, in this part of the river, and in order to favor the transport of organic matter to the agricultural valleys. At Thac Buoi, organic phosphorus concentrations are very high, often from two to four times higher than the concentrations upstream and downstream (see figure 8). This can be observed in all seasons and could be due to the release of organic phosphorus from the agricultural lands, either from rice fields or directly from the sedimentary deposits that are highly biologically active. This is why a negative value was given to σ_5 in the central region ($\sigma_5 = -0.05 \text{ d}^{-1}$), reflecting a benthic contribution in organic phosphorus in this agricultural area. Some studies have shown that organic phosphorus can be transported with suspended sediments (e.g. SHEN *et al.*, 2008)

and this is what was observed for the Cau River in January (see figure 5). Observations at Thac Buoi show the importance of the organic phosphorus availability in this agricultural region rich in alluvium. At Gia Bay, the concentrations of organic phosphorus are generally lower. It can be presumed that the settling rate of organic P is very high in this region (a value of $\sigma_5 = 1 \text{ d}^{-1}$ was chosen) due to the deposition of suspended sediments in this region where the river flow velocity is reduced.

Many local reports mention ammonia odors along the riverbank near Gia Bay. Moreover, denitrification, and thus production of nitrogen gas N_2 , could occur in this area when concentrations in dissolved oxygen are low. This means that there could be a net loss of nitrogen to the atmosphere, which is not taken into account in the model. Indeed, in QUAL2E and QUAL-GIBSI, the denitrification process is not simulated, but the nitrification module is stopped when concentrations in dissolved oxygen are low. To take this into account, negative values were given to σ_3 , the benthic ammonium source rate in the three regions ($-0.1 \text{ mg N}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$ in Region I, $-0.5 \text{ mg N}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$ in Region II, and $1 \text{ mg N}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$ in Region III). Negative values of σ_3 allow to reproduce nitrogen losses in the model, losses that could occur either by deposition of suspended solids or by ammonia or N_2 losses to the atmosphere.

Finally, for the calibration of σ_4 , the settling rate of organic N, it was assumed to be minimal upstream ($\sigma_4 = 0.001 \text{ d}^{-1}$ in Region I) and maximal downstream ($\sigma_4 = 0.1 \text{ d}^{-1}$ in Region III) according to the physical characteristics of each environment. However, in Region II, input loads from agriculture could counterbalance the deposition rate and thus a minimal value for σ_4 was retained ($\sigma_4 = 0.001 \text{ d}^{-1}$ in Region II).

All these considerations show how a comprehensive study of land use and land physical characteristics, in conjunction with observed data, can help to estimate the regional values of the model's parameters. This approach could be beneficial for river water quality modelling on any type of watershed, and especially on those where observed data are too scarce to describe all the dynamics related to water quality, like often encountered in developing countries. It also shows how a judicious definition of the value of some parameters allows reproducing processes that are not explicitly represented in the model (e.g. oxygen demand for the degradation of coliforms, denitrification and production of nitrogen gas).

4. CONCLUSION

A novel methodology for the calibration of water quality simulation models, which applies to large watersheds where intensive measurements for water quality and quantity are

lacking, was proposed in this paper. The methodology is based on: 1) the use of the results from a hydrological model to provide the required hydrological variables (discharge, water level and velocity) to the water quality model; 2) five assumptions for the definition of initial and boundary conditions; 3) a three-step regionalized calibration method, in which the specific characteristics of the different subwatersheds are taken into account and 4) the adjustment of some parameters in order to reproduce processes that are not explicitly represented in the model. The methodology was applied, as a test case study, to the Cau River in Vietnam. As compared to most of the calibration studies that were previously conducted on river water quality models with optimization algorithms, the proposed procedure relies on a comprehensive study of the land use and characteristics on each subwatershed and the definition of different sets of parameters values in distinct regions. For the specific case of the Cau River, the sensitivity analysis, that is part of the calibration method, showed that the parameters to which the model's results are the most sensitive are: β_1 and β_2 for nitrites; μ and σ_1 for chlorophyll *a*; β_1 for ammonium; K_3 for BOD_5 ; and K_2 for DO. These results could guide future calibration work for river water quality models in the South East Asia Region, or in any other watershed experiencing a tropical monsoon climate. Application of the methodology to the Cau River also showed that calibration and validation results were significantly improved by applying regionalization as compared to an initial calibration for which a single set of parameters values was used for the whole simulated river stretch. Furthermore, use of the results from a hydrological model to provide the required hydrological variables to the water quality model demonstrates how integrated modeling systems at the watershed scale, by combining different simulation models, can be beneficially applied on watersheds where observed data are scarce. When integrated in such an integrated modeling system, the river water quality model, once calibrated, can be used in conjunction with other simulation models at the watershed scale (as for example, pollutant and/or sediment production and transport models) to assess the impacts of various potential future interventions on the river water quality.

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APPENDIX 1

This appendix presents a summary of some reaction equations in QUAL2E. The complete equations are presented in BROWN and BARNWELL (1987).

Dissolved oxygen

$$\frac{dO}{dt} = K_2(O_s - O) + (\alpha_3\mu - \alpha_4\rho)A - K_1L - \frac{K_4}{d} - \alpha_5\beta_1N_1 - \alpha_6\beta_2N_2 \quad (\text{A-1})$$

Reaeration rate

Option 2, CHURCHILL et al. (1962):

$$K_2 = 11.6 \frac{\bar{u}^{-0.969}}{d^{1.673}} \quad (\text{A-2})$$

with \bar{u} in $\text{ft}\cdot\text{s}^{-1}$ and d in ft.

Option 3, O'CONNOR and DOBBINS (1958):

$$K_2 = 45 \frac{\bar{u}^{-0.5}}{d^{1.5}} \quad (\text{A-3})$$

with \bar{u} in $\text{ft}\cdot\text{s}^{-1}$ and d in ft.

Carbonaceous BOD

$$\frac{dL}{dt} = -K_1L - K_3L \quad (\text{A-4})$$

$$L = 1.46\text{BOD}_5 \quad (\text{A-5})$$

Coliforms

$$\frac{dE}{dt} = -K_5E \quad (\text{A-6})$$

Chlorophyll-A

$$\text{Chla} = \alpha_0A \quad (\text{A-7})$$

$$\frac{dA}{dt} = \mu A - \rho A - \frac{\sigma_1}{d}A \quad (\text{A-8})$$

Ammonia nitrogen

$$\frac{dN_1}{dt} = \beta_3N_4 - \beta_1N_1 + \frac{\sigma_3}{d} - F\alpha_1\mu A \quad (\text{A-9})$$

Nitrite nitrogen

$$\frac{dN_2}{dt} = \beta_1N_1 - \beta_2N_2 \quad (\text{A-10})$$

Nitrate nitrogen

$$\frac{dN_3}{dt} = \beta_2N_2 - (1-F)\alpha_1\mu A \quad (\text{A-11})$$

Organic nitrogen

$$\frac{dN_4}{dt} = \alpha_1\rho A - \beta_3N_4 - \sigma_4N_4 \quad (\text{A-12})$$

Organic phosphorus

$$\frac{dP_1}{dt} = \alpha_2\rho A - \beta_4P_1 \quad (\text{A-13})$$

Dissolved phosphorus

$$\frac{dP_2}{dt} = \beta_4P_1 + \frac{\sigma_2}{d} - \alpha_2\mu A \quad (\text{A-14})$$

APPENDIX 2

List of symbols

A	algal biomass concentration ($\text{mg } A \cdot \text{L}^{-1}$)
BOD_5	5-day BOD ($\text{mg} \cdot \text{L}^{-1}$)
$\text{Chl}a$	chlorophyll a concentration ($\mu\text{g Chl}a \cdot \text{L}^{-1}$)
d	mean stream depth (m)
E	concentration of coliforms (colonies/100 ml)
F	fraction of algal N uptake from ammonium pool
K_1	BOD decay rate (d^{-1})
K_2	reaeration rate (d^{-1})
K_3	BOD settling rate (d^{-1})
K_4	SOD (sediment oxygen demand) uptake rate ($\text{mg O} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$)
K_5	coliform decay rate (d^{-1})
L	ultimate BOD ($\text{mg} \cdot \text{L}^{-1}$)
N_1	ammonia nitrogen concentration ($\text{mg N} \cdot \text{L}^{-1}$)
N_2	nitrite nitrogen concentration ($\text{mg N} \cdot \text{L}^{-1}$)
N_3	nitrate nitrogen concentration ($\text{mg N} \cdot \text{L}^{-1}$)
N_4	organic nitrogen concentration ($\text{mg N} \cdot \text{L}^{-1}$)
P_1	organic phosphorus concentration ($\text{mg P} \cdot \text{L}^{-1}$)
P_2	inorganic or dissolved phosphorus concentration ($\text{mg P} \cdot \text{L}^{-1}$)
O	concentration of dissolved oxygen ($\text{mg} \cdot \text{L}^{-1}$)
O_s	saturation concentration of dissolved oxygen ($\text{mg} \cdot \text{L}^{-1}$)
\bar{u}	average velocity in the stream ($\text{m} \cdot \text{s}^{-1}$)
α_0	ratio of chlorophyll a to algal biomass
β_1	ammonium decay rate (d^{-1})
β_2	nitrite decay rate (d^{-1})
β_3	organic N decay rate (d^{-1})
β_4	organic P decay rate (d^{-1})
μ	algal growth rate (d^{-1})
ρ	algal respiration rate (d^{-1})
σ_1	algal settling rate ($\text{m} \cdot \text{d}^{-1}$)
σ_2	benthic dissolved P source rate ($\text{mg P} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$)
σ_3	benthic ammonium source rate ($\text{mg N} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$)
σ_4	organic N settling rate (d^{-1})
σ_5	organic P settling rate (d^{-1})

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