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BACTERIAL MODELLING OF A RURAL TROPICAL STREAM USING THE QUAL2K MODEL

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Abstract: Previous studies showed that the Serin River and its tributaries water and sediment were contaminated with *Escherichia coli* (*E. coli*) due to human activities along the river. Since the water of this river is important as a source of drinking water, body contact recreation, laundry and fish culture, it is important that *E. coli* count be kept at a safe level for the health of the communities. Therefore, the objective of this study is to utilize the water quality model to simulate *E. coli* concentration in the river water for its designated use. The QUAL2K model was calibrated and validated using field data from October 2009 to March 2010. The results showed that 80% of the predicted concentrations fall in the range of the observed values. Subsequently, the model was applied to simulate two different scenarios of designated use. The model simulation results showed that for the river water to be suitable as drinking water, no *E. coli* should be discharged from the headwater and from Bukah tributary. As for the suitability of the river water for recreational purposes, the maximum allowable concentrations of *E. coli* for the headwater, and the following tributaries, namely, the Bukah River, Pam River and Bukar River were 400 CFU/100mL, 900 CFU/100mL, 1000 CFU/100mL and 380 CFU/100mL respectively during low water level. During high water level, the maximum allowable concentrations from those tributaries are higher than that during low level due to increased dilution.

KEYWORDS: Water quality modelling, Serin River, *E. coli*, QUAL2K.

Introduction

Surface water is frequently contaminated by microorganisms from different sources such as farm animals and agriculture (Hyland *et al.,* 2003; Pappas *et al.,* 2008; Muyibi *et al.,* 2008; Mishra *et al.,* 2008), sewage (Gerba & Smith, 2005; Muyibi *et al.,* 2008) and wild animals (Jiang *et al.,* 2007). Contamination of surface water renders the water unsuitable for its designated purposes such as drinking, body contact recreation and it affects fish and shellfish quality due to the potential for human to be infected by pathogens. It has been reported that majority of diarrhoeal disease in the world (88%) and approximately 1.7 million deaths worldwide was attributable to unsafe water, sanitation and hygiene (WHO, 2003). In developing regions, drinking water is a major source of microbial pathogens (Ashbolt, 2004). Sewage exposed fish has been found to harbour drug resistant coliforms (Sanyal *et al.,* 2011). The Serin River, a rural river located in south-western part of Sarawak, is an important river for the communities around the area. Its importance includes a drinking water source, fish aquaculture, laundry and recreation. But, landuse and settlement in the river basin have contributed to water quality contamination. Previous studies showed that the water and sediment along the river are contaminated with *E. coli* and levels are high near human settlement and animal farms (Ling *et al.,* 2006; 2008; 2012; 2013). In order to reduce the contaminants so that the water is suitable for use according to its designated purposes, it is best that modelling be applied. In Malaysia, fecal coliform limit of National Water Standards for Class I (no treatment required), IIA and IIB are 10 count/100mL, 100 count/100mL and 400 counts/100mL respectively.

Water quality modelling is useful for predicting pollutant and contaminant concentrations in rivers for water quality management. Bougeard *et al.,* (2011) applied modelling approach to calculate *E. coli* concentrations in estuarine water and shellfish. The QUAL2K is a modernized version of QUAL2E model that was developed by Brown & Barnwell (1987). The QUAL2E and QUAL2K models have been used extensively to simulate surface water quality (McCutcheon, 1989; Chapra, 1997; Park *et al.,* 2002; Paliwal *et al.,* 2007; Fang *et al.,* 2008) and they are able to simulate up to 15 different water quality parameters. Mohamed (2001) applied QUAL2E model to simulate water quality parameters in a river in West Malaysia. Hohls *et al.,* (1995), Steynberg *et al.,* (1995) and Venter *et al.,* (1997) used QUAL2E model to simulate microbial water quality. DNR (2007) used QUAL2K to measure total maximum loads for *E. coli*. The QUAL2K model is a one dimensional model where river channel is assumed to be well-mixed vertically and laterally. It employs steady state hydraulics, uses diel heat budget and calculates diel water-quality kinetics (Chapra *et al.,* 2007). It simulates a river by representing a river as a series of reaches which have constant hydraulics characteristics and these reaches can be further divided into a series of elements. In QUAL2E model, temperature dependent die-off rate of bacteria was used whereas in QUAL2K model, two extra functions were added which are the light dependent die-off rate and the pathogen settling effect which gave a more comprehensive approach on determining the bacterial die-off rate. Since the Serin River is well-mixed, in this work, QUAL2K model was used to simulate *E. coli* concentrations.

Data and Modelling

Data Collection and Segmentation

Data needed as input to the model were collected at the site. The study site, *in-situ* parameters measurements (temperature and pH), water samples collection, total suspended solids (TSS) and *E. coli* analyses have been

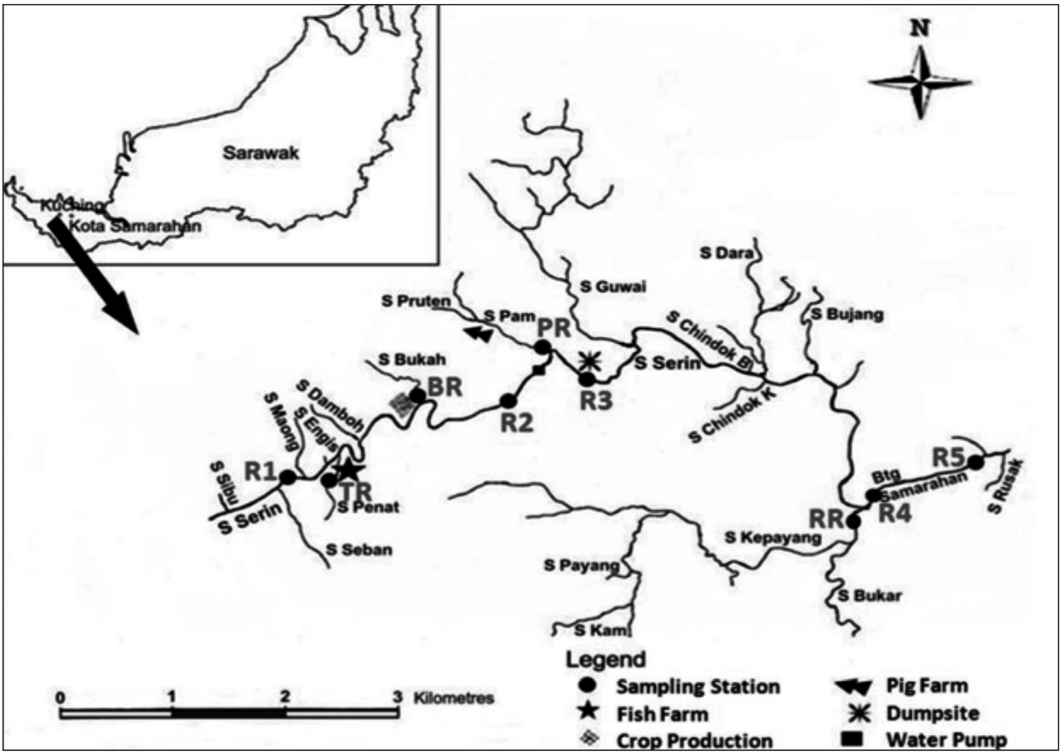

Figure 1: The Location of Each Sampling Stations and Human Activities along the River

Table 1: Descriptions of the Sampling Stations along the Serin River

Station	Description
R1	Headwater, upstream next to Ma'ang village and a primary school
TR	Downstream of fish pond discharge
BR	Animal farming upstream and subsistence farming
R2	Received discharge from BR
PR	Received lagoon discharge from pig farming
R3	Downstream of SP and near a dumping site
RR	Downstream of Kampung Taie and received runoff from oil palm plantation
R4	Received high volume discharge from RR
R5	Downstream, residential areas along the station and next to Kuching-Serian highway

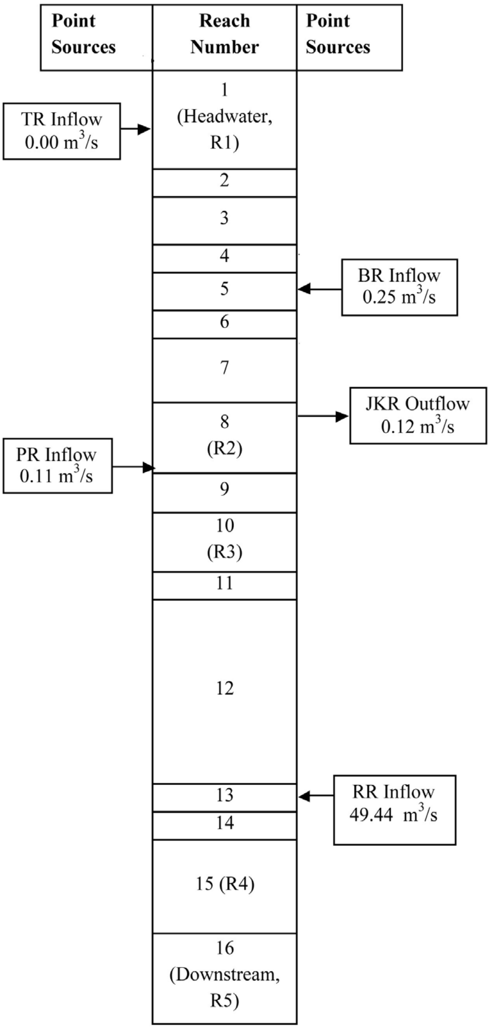

Figure 2: Segmentation of Serin River for QUAL2K Model Application

described in Ling *et al.,* (2013). The map of the study site with stations studied in the main river and tributaries is also shown in Figure 1 and Table 1 gives the description of the stations. Solar radiation was measured *in-situ* using a pyranometer (Silicon 3670) and a data logger (Watchdog 400). The geometric characteristics of the river was measured with a depth finder (Hondex, PS-7 LCD Digital Sounder) and a range finder (Bushnell, Elite 1500), while the velocity of the water was determined using a flow meter (Flo-Mate 2000). The segment of the river studied was divided into 16 reaches. Figure 1 shows the schematic diagram of the segmented river. Outflow as in water abstraction by Sarawak Public Works Department (JKR) is conducted at km 6.7 at the rate of 0.12 m^3/s. *E. coli* concentrations obtained from sampling stations at the tributaries and the cross-sectional area and flow provided inputs on the loadings from tributaries.

Computation of Die-off Rate

Bacterial loss in the river water, also called die-off is an important parameter to be estimated. Factors that affect die-off include physical factors such as sedimentation, temperature and adsorption; physicochemical factors such as pH and osmotic effects; and lastly, biochemical-biological factors such as nutrient levels and presence of predators (Bowie *et al.,* 1985). In QUAL2K model, the total bacteria die-off rate is dependent on base mortality rate, loss rate due to solar radiation and settling loss rate as shown in equation (2) (Chapra, 1997);

$$k'_b = k_{b1} + k_{bi} + k_{bs} \tag{2}$$

where k'_b is the total loss rate (d^{-1}), and k_{b1} is the base mortality rate (d^{-1}), k_{bi} is the loss rate due to solar radiation (d^{-1}), and k_{bs} is the settling loss rate (d^{-1}).

Base mortality loss, k_{b1}, is a measure of natural die-off and is expressed as first order decay dependent on temperature (Ling *et al.,* 2005) and salinity and it is adopted from Mancini (1978) as stated in (Chapra, 1997). k_{b1} is calculated using equation (3);

$$k'_1 = (0.8+0.02S)1.07^{T-20} \tag{3}$$

where S is salinity (g/L), and T is temperature (°C) where both were measured on site.

Effect of solar radiation on bacterial die-off has been studied. According to Richard *et al.,* (2004), insolation primarily inactivated *E. coli* and it was shown that *E. coli* count during morning were significantly higher compared to that in the afternoon and cloudy days often had higher counts than sunny days. In this model, k_{b1} is computed using equation (4);

$$k'_i = \frac{\propto l_0}{k_e H}(1-e^{-keH}) \tag{4}$$

where $\propto$ is a proportionality constant, that is, light efficiency factor where the value used was 1 (Chapra, 1997). l_0 is the surface light energy (ly/hr), k_e is the extinction coefficient (m^{-1}), and H is the depth of water (m).

Bacteria has been found to adsorb to soil particles (Ling *et al*., 2002) and settle (Hipsey *et al.,* 2006) and thus result in decreased time in suspension (Fries *et al.,* 2006). k_{bs} is computed using equation (5);

$$k'_s = F_p \frac{v_s}{H} \tag{5}$$

where F_p is the fraction of the bacteria that are attached, and v_s is the settling velocity of particles (m/d).

Substituting equations (3), (4) and (5) into equation (1) gives the total bacteria die-off rate which can be expressed as equation (6);

$$k'_b = (0.8+0.02S)1.07^{T-20} + \frac{\alpha l_0}{k_e H}(1-e^{-keH}) + F_p \frac{v_s}{H} \tag{6}$$

$$k_e = 0.55*\text{TSS} \tag{7}$$

$$F_p = \frac{k_d TSS}{1+k_d TSS} \tag{8}$$

where k_e is proportional to TSS, which is the total suspended solids (mg/L) the values of which were obtained from sample analysis. The values of k_d and v_s used were 0.01 and 8.64 respectively (Bai & Lung, 2005).

Model Calibration and Validation

The QUAL2K model was calibrated and validated into two different conditions to simulate the high and low flow conditions of the river water. Once the model had been validated, the model was used to predict the maximum amount of pollutants that can be discharged into the river to qualify for Class I and Class IIB respectively where the standards were set up by NWQS. Table 2 showed the dates of data collection that were used for model calibration and validation.

Table 2: Dates of Data Collection and Sampling Stations Data for Calibration and Validation

Sampling Date	Sampling Stations	Remarks
26 October 2009	R1, TR, BR, R2, PR, R3, RR, R5	Calibration
8 December 2009	R1, TR, BR, R2, PR, R3, RR, R5	Validation
19 January 2010	R1, R2, R3, R5	Calibration
1 February 2010	R1, R2, R3, R5	Validation
24 February 2010	R1, R2, R3, R5	Calibration
10 March 2010	R1, TR, BR, R2, PR, R3, RR, R5	Validation

During calibration, the reaction rates and coefficients were adjusted so that simulated data and field data were in agreement. Reaction coefficients such as particle settling velocity and partition coefficient were adopted from literatures (Bai & Lung, 2005; Rehmann & Soupir, 2009). For other reaction coefficients that were not provided in those studies, default values in the model were used. Table 3 summarizes the values of reaction coefficients that were adopted. The *E. coli* concentration entered into the data was in

Table 3: Reaction Coefficients that were Adopted for Use in QUAL2K Model

Parameter	Symbol	Unit	Reference Range	Adopted Value
Settling velocity	V_s	m/d	8.64a-803.52b	8.64a
Partition Coefficient	K_d	m^3/g	-	0.01a
Temperature Correction	Θ_{dx}	Dimensionless	1.024-1.08[c]	1.07[c]
Pathogen Light Efficiency Factor	α_{path}	Dimensionless	-	1[c]

Sources: [a] Bai & Lung (2005) [b] Rehmann & Soupir (2009) [c] Chapra (1997)

Table 4: Diffuse Flow and Non-point *E. coli* Sources Obtained from Model Calibration

Location (km)	Diffuse Flow and Non-point *E. coli* Sources			
	Low Flow		High Flow	
	Flow (m^3/s)	*E. coli* (CFU/100mL)	Flow (m^3/s)	*E. coli* (CFU/100mL)
6.10	20	2000	50	3000
4.95	10	2000	5	5000
4.75	15	3000	20	14000

CFU/100mL unit. Data such as air temperature, dew point temperature, shade percentage, hourly cloud cover and hourly wind speed were obtained from the Meteorological Services Department, Kuching. Once the reaction rates and coefficients were determined, the values were used for validation with a new set of field data.

Several assumptions were made in calibration and validation. They are, *E. coli* concentration input for headwater was similar for both model calibration and model validation; the flow and *E. coli* concentrations from all the tributaries were kept similar for both model calibration and model validation; and diffuse flows and non-point *E. coli* sources were assumed to occur and values obtained by calibration and kept similar for both model calibration and model validation (Table 4) because it was observed that there were several non-point sources pollution that could be identified in the study area.

Results and Discussion

Die-off Rate

Computed values of temperature dependent die-off rate of *E. coli*, solar radiation dependent die-off rate of *E. coli* and settling dependent die-off rate of *E. coli* of each sampling stations are shown in Table 5, Table 6 and Table 7 respectively. The total *E. coli* die-off rate of each sampling station is shown in Table 8 where the total die-off rate chosen for model input was 2.15 d^{-1}. The die-off rate chosen was relatively higher than the die-off rate of *E. coli* (0.340 ± 0.012 d^{-1}) reported in Ling *et al.,* (2008) using Serin River water because it might be due to the fact that the decay rate reported was conducted in a control environment in the laboratory where several factors such as solar radiation and settling effect were not taken into account.

Calibration

Table 9 shows the loadings from tributaries for model calibration and validation during low water and high water levels. The calibration results are displayed in Figures 3 and 4. The water flow fitted the observed data well. For simulation of *E. coli* concentrations, there was a small increase of concentration at km 8.1 due to inflow from BR which received animal farm effluent upstream that recorded quite high concentration of *E. coli*. The *E. coli* concentration decreased as water moved downstream due to dilution but there was a sudden surge of *E. coli* concentration around km 6. This was the response to inflow from PR which received pig farm effluent and flow from diffuse source into the river between R2 and R3. Bitton (1994) reported that feces matter can contain up to $1x10^{12}$ bacteria per gram and average *E. coli* were $3.3x10^{6}$ per gram of pig's feces. The impact of animal farms effluent on the *E. coli* concentrations in those two tributaries, BR and PR, has been reported by Ling *et al.,* (2006) and the concentrations ranged from to be 400-12,000 CFU/100mL and 4,000-1,000,000 CFU/100mL respectively. The *E. coli* concentration in the Serin River was between 2,000 and 6,000 CFU/ 100mL and that was much lower than the concentration from PR which was the highest (69,100 CFU/100mL) among all the tributaries (Table 9). This is due to the low flow into the main river which was only 0.11 m^3/s. Then, the *E. coli* concentration started to decrease again due to dilution until km 5.9 after which the *E. coli* concentration remained quite constant. At km 2.96, the concentration of *E. coli* increased drastically due to input from RR which received agricultural run-off and domestic wastes and diffuse sources. Even though the *E. coli* concentration detected at RR was lower compared BR and RR tributaries (Table 9), the volume of water flowing into the main river was the highest among all the tributaries, 49.44 m^3/s. During high water level, the *E. coli* concentrations are higher than low water level due to diffuse sources and the PR and RR inputs have less impact with smaller surges. Overall, the model was able to calibrate well for both low water and high water conditions of the Serin River.

Table 5: Temperature Dependent Die-off Rate of *E. coli* Using Equation (3)

Station	**Temperature Dependent Die-off Rate** $k'_b = (0.8+0.02S)1.07^{T-20}$		
	Salinity (g/L)	***Temperature (°C)***	**(d^{-1})**
R1	0	24.85	1.11
TR	0	26.59	1.25
BR	0	26.16	1.21
R2	0	25.85	1.19
PR	0	25.84	1.19
R3	0	25.93	1.19
RR	0	26.23	1.22
R4	0	26.88	1.27
R5	0	26.26	1.22

Table 6: Solar Radiation Dependent Die-off Rate of *E. coli* Using Equation (4)

Station	**Temperature Dependent Die-off Rate** $k'_i = \frac{\propto l_0}{k_e H}(1-e^{-keH})$				
	$\propto$	l_0 **(ly/hr)**	k_e**(m^{-1})**	H**(m)**	k_{bi}**(m^{-1})**
R1	1	10.11	7.24	1.15	1.21
TR	1	16.95	6.25	0.39	6.35
BR	1	7.3	19.27	0.34	1.11
R2	1	11.45	4.48	1.01	2.50
PR	1	46.33	31.37	0.33	4.48
R3	1	6.74	6.89	1.79	0.48
RR	1	29.74	14.89	2.06	0.97
R4	1	18.02	11.48	3.46	0.45
R5	0	23.29	15.23	2.78	0.55

Table 7: Settling Dependent Die-off Rate of *E. coli* Using Equation (5)

Station	**Temperature Dependent Die-off Rate** $k'_{bs} = F_p \frac{v_s}{H}$			
	F_p	v_s **(md^{-1})**	H**(m)**	k_{bs}**(d^{-1})**
R1	0.12	8.64	1.15	0.87
TR	0.10	8.64	0.39	2.26
BR	0.26	8.64	0.34	6.58
R2	0.08	8.64	1.01	0.64
PR	0.36	8.64	0.33	9.50
R3	0.11	8.64	1.79	0.53
RR	0.21	8.64	2.06	0.88
R4	0.17	8.64	3.46	0.43
R5	0.22	8.64	2.78	0.67

Table 8: Die-off Rates of *E. coli* Using Equation (6)

Station	**Die-off Rate** $k'_b = k_{b1} + k_{bi} + k_{bs}$			
	k_{b1}	k_{bi}	k_{bs}	k'_b
R1	1.11	1.21	0.87	3.19
TR	1.25	6.35	2.26	9.86
BR	1.21	1.11	6.58	8.90
R2	1.19	2.50	0.64	4.33
PR	1.19	4.48	9.50	15.17
R3	1.19	0.48	0.53	2.19
RR	1.22	0.97	0.88	3.07
R4	1.27	0.45	0.43	2.15
R5	1.22	0.55	0.67	2.44

Table 9: Observed Flow and *E. coli* Concentrations from Tributaries for Model Calibration and Validation and Predicted Maximum Allowable Concentrations of *E. coli* for Class IIB Compliance

Station	**Observed flow and *E. coli* from tributaries**		**Predicted maximum allowable *E. coli***	
	Flow (m^3/s)	***E. coli* (CFU/100mL)**	**Low Water (CFU/100mL)**	**High Water (CFU/100mL)**
TR	0.00	3000	0	0
BR	0.25	15500	900	1600
PR	0.11	69100	1000	2500
RR	49.44	5700	380	510

Validation

The inflow of *E. coli* concentration for model validation from each tributary was kept similar to that of model calibration as given in Table 9. The validated results are shown in Figure 5 for low water and Figure 6 for high water levels. Figure 5 and 6 showed similar trend when compared to calibrated results. In general, the simulated *E. coli* concentrations during low water condition and high water condition were within the maximum and minimum range of observed *E. coli* concentrations. However, the observed concentration of *E. coli* at R3 was higher than the predicted concentrations for both high water and low water levels during calibration and validation. In QUAL2K model, mean value of inflow *E. coli* from tributaries was used as input. It is possible that there was larger load from the PR tributary than that detected during sample collection which occurred in the late morning as Ling *et al.,* (2008) reported that during hourly sampling from 8:30 am to 4:30 pm, *E. coli* concentrations fluctuated with lowest counts between 8:30 am-11:30 am and the highest counts at 12:30 pm and 1:30 pm. It is also possible that sediment associated *E. coli* from resuspension contributed to the observed *E. coli* at station R3 as sediment *E. coli* study at those stations showed that sediment at R3 has higher concentration than R2 and R4 67% of the sampling times (Ling *et al*., 2012) whereas the model only consider input from tributaries, but not the re-suspension of sediment in the river.

Application of Model

For drinking water purposes, NWQS has set 10 CFU/100mL as the standard for Class I (DOE, 2008), which is suitable for using river water as drinking water source. From the prediction result (Figure 7), it could be seen that the input from BR was to remain 0 CFU/100mL and any diffuse sources input was also set to remain 0 CFU/100mL for the simulated *E. coli* concentration to remain below 10 CFU/100mL. It is important so that the water abstraction point at km 6.7 would abstract the kind of quality of river water that required no necessary treatment for drinking water.

As most of the villagers use the Serin River for daily uses such as bathing, especially near the headwater and R5 where there were housing areas situated along the river, there is a need to predict the amount of *E. coli* contamination that is allowed for the river water to adhere to the quality set up by NWQS. NWQS has set 400 CFU/100mL to qualify for Class IIB where recreational use with body contact is suitable (DOE, 2008). Figure 8 shows that the model was able to predict the concentration of *E. coli* for compliance. *E. coli* concentrations from each of the tributaries must be significantly reduced so that the simulated concentrations of *E. coli* do not exceed the 400 CFU/100mL limit. Table 9 summarizes the maximum allowable inflow concentrations of *E. coli* of each tributary for compliance. During high water, higher allowable concentrations of *E. coli* are possible without exceeding the 400 CFU/100mL limit because higher flow during high water would result in higher dilution of the *E. coli* concentration. PR could discharge higher concentration of *E. coli* compared to other tributaries such as BR (0.25 m^3/s) and RR (49.44 m^3/s) because the flow into the main river was lower (0.11 m^3/s).

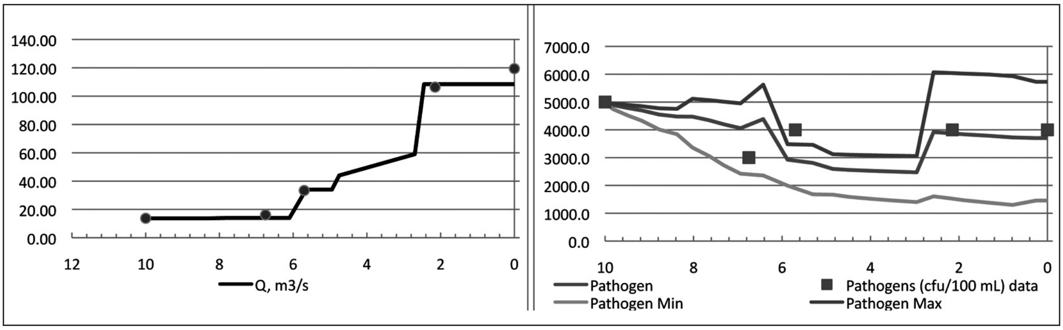

Figure 3: Calibration Results of Flow and *E. coli* Concentrations During Low Water of the Serin River Using QUAL2K Model

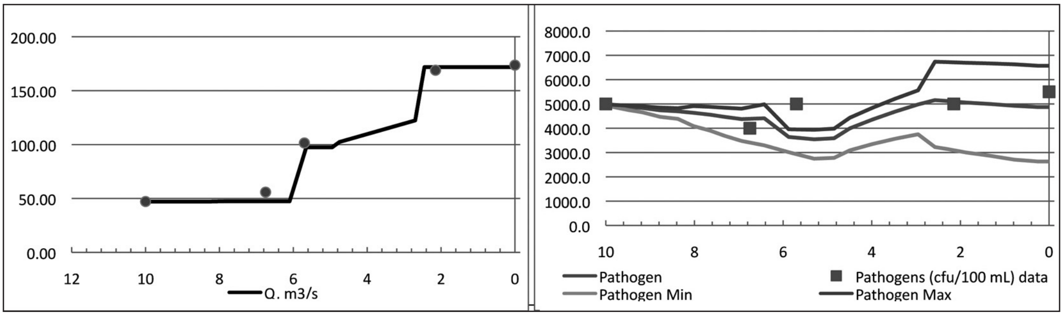

Figure 4: Calibration Results of Flow and *E. coli* Concentrations During High Water of the Serin River Using QUAL2K model

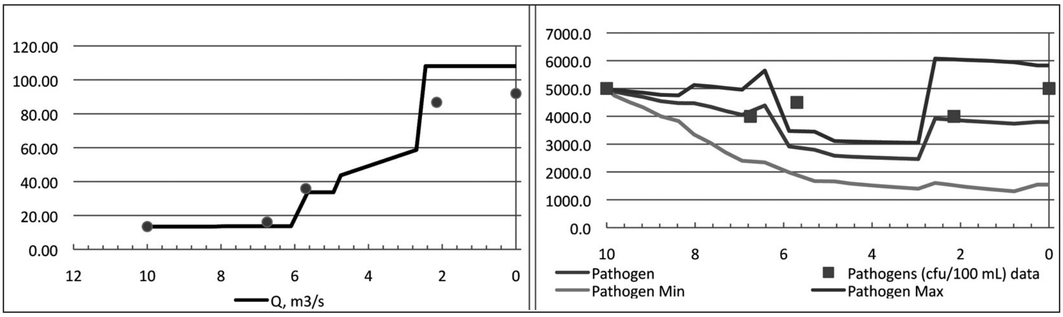

Figure 5: Validation Results of Flow and *E. coli* Concentrations During Low Water of the Serin River using QUAL2K Model

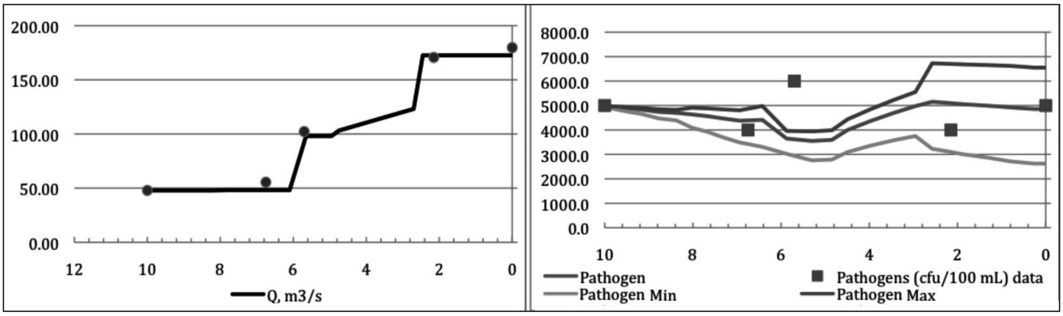

Figure 6: Validation Results of Flow and *E. coli* Concentrations During High Water of the Serin River Using QUAL2K Model

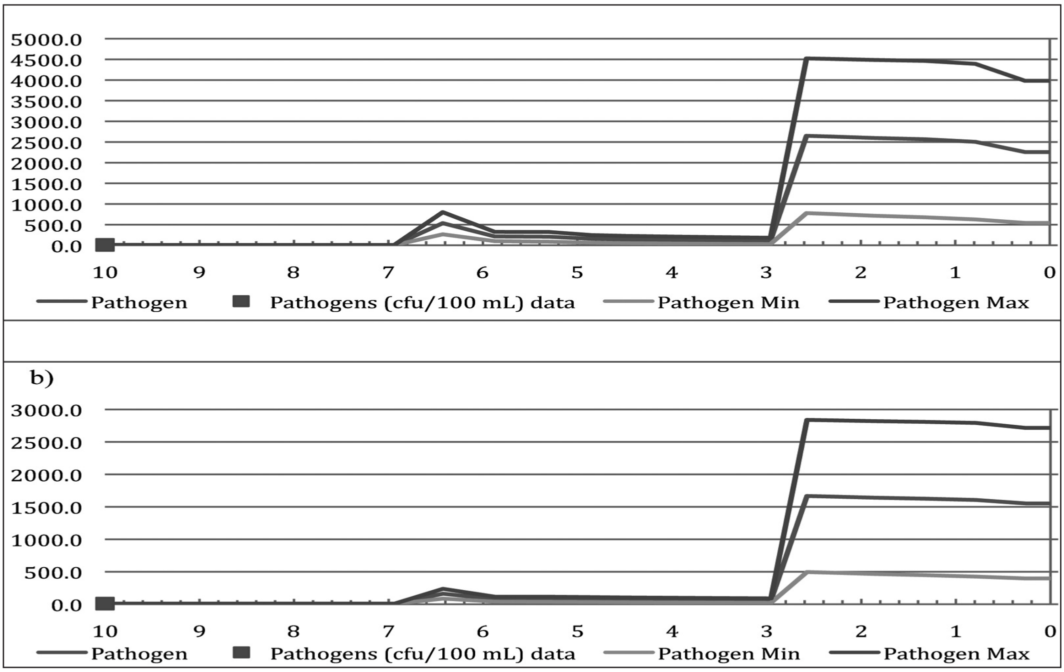

Figure 7: Prediction Results of *E. coli* Concentration for Drinking Water Source without Input from Bukah River of the Serin River Using QUAL2K Model; a) During Low Water and b) During High Water

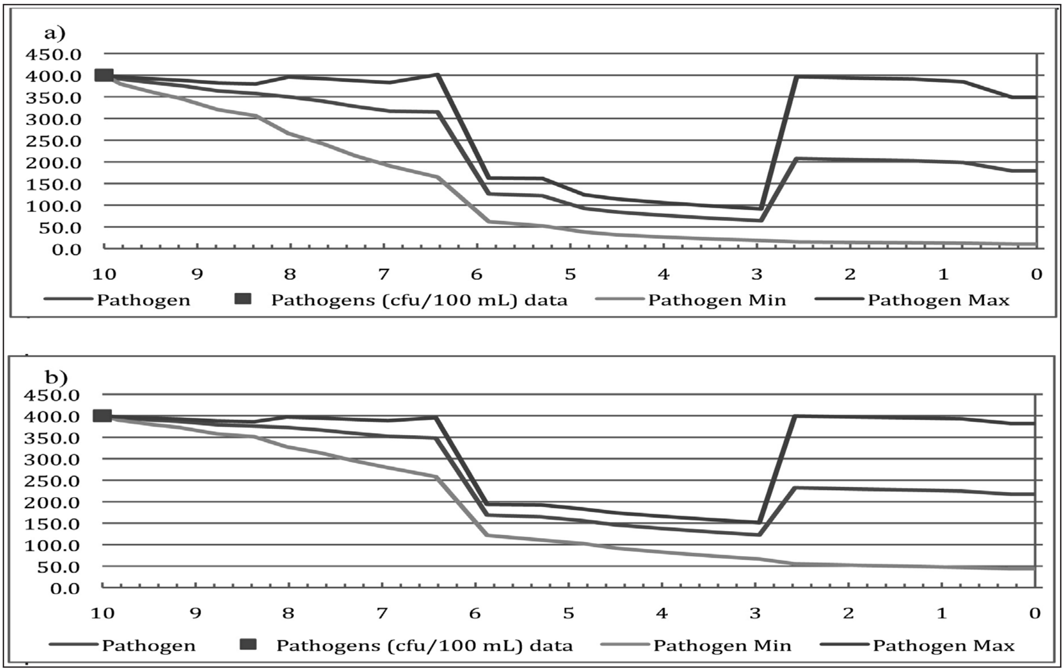

Figure 8: Prediction Results of *E. coli* Concentration of the Serin River for Recreational Purposes Using QUAL2K model: a) During Low Water and b) During High Water

Conclusion

The model was calibrated and validated for prediction of *E. coli* concentration in the river water with 80% of the simulated concentrations within minimum and maximum observed concentrations. It was found that the flow and die-off rate of *E. coli* had significant impact on the simulation of *E. coli* concentrations in the river. Prediction results showed that no *E. coli* contamination from headwater and Bukah River was permitted for the river water to be suitable for drinking. Significant reduction in *E. coli* contamination from each of the tributaries had to occur for the river water to comply with Class IIB standard for body contact recreation. Further research needs to be carried out to determine other factors that affect the *E. coli* concentration in the river such as re-suspension of *E. coli* from sediment and diffuse sources. In addition, proper treatment and management of animal wastes and agricultural run-off need to be carried out to minimize the impact on water resources.

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