Research Paper

Numerical modelling of FC bacteria using a dynamic and variable mortality rate

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ABSTRACT

Faecal coliform (FC) microorganisms are one of the most important indicators in water quality management, since their presence reveals the possibility of existence of other dangerous microorganisms, leading to higher health risks. An accurate estimate of the concentration of this indicator helps better evaluation of the water pollution in riverine basins; thus, it is essential for future developments. The FC mortality rate depends on the physical, chemical, and biological processes in rivers. These processes are generally affected by environmental conditions. In this study, the decay coefficient (K) or mortality rate are related to the environmental parameters such as temperature, turbidity, pH, and salinity by an empirical equation. The results showed that turbidity and temperature are the most effective parameters. Moreover, an empirical equation was developed utilizing numerical model calibration, which describes the relationship of the mortality rate (K) with water temperature and turbidity. This equation was then added to the water quality module of the FASTER numerical model. Comparison of the measured FC concentrations with the predicted values obtained from the numerical model showed that the model accuracy significantly improved for the dynamic and variable decay coefficient.

Key words | biological water pollution, environment, faecal coliform, mathematical modelling, river engineering

HIGHLIGHTS

- New method for modelling faecal coliform bacteria (FCB).
- Dependence of faecal coliform mortality rate to environmental factors.
- Dynamic and variable faecal coliform decay coefficient.
- More accuracy for prediction of faecal coliform concentration.
INTRODUCTION

Biological pollution in water bodies, e.g. streams, rivers, lakes, reservoirs, estuaries, and seas, is usually recognized by the existence of any types of microorganisms and bacteria. Some kinds of bacteria are perilous for human health. Faecal coliform (FC) is a kind of bacteria living in the intestine of warm-blooded animals. It is an indicator of biological water pollution, for instance, its existence in the water body depicts the amount of the biological water pollution (USEPA 1986). Numerical models are generally beneficial for dynamic modelling of the flow and water quality in different water bodies. However, an accurate prediction of the pollutant concentrations enables the environmental managers and authorities to make the proper decisions for future developments. The accuracy of the numerical solution of the governing partial differential equations for flow and water quality is highly dependent on the precise estimations of the empirical coefficients involved. In the numerical modelling of FC, the accurate estimation of the bacterial mortality rate or decay coefficient is essential for accurate predictions of its spatial and temporal concentration. In many commercial numerical models, this coefficient is assumed to be constant at any point and along the whole simulation time. Many researchers have found that the mortality rate is not constant; in addition, due to different environmental factors such as salinity, turbidity, sediment concentration, temperature and pH, the decay coefficient may vary within a wide range (0.001 h⁻¹ to more than 100.0 h⁻¹). Therefore, a
variable decay coefficient or mortality rate based on the environmental parameters leads to the more accurate prediction of the FC concentration.

The main aim of this study is to investigate the effect of environmental parameters, such as water temperature and turbidity, on the mortality rate or decay coefficient of faecal indicators utilizing numerical model calibration and verification. A new procedure will be described to produce a dynamic mortality rate, and taking advantage of this modified decay coefficient it can be possible to significantly improve the predicted faecal coliform concentrations in riverine basins. A review of the literature shows that most equations are introduced by researchers in order to find a relationship between some environmental parameters and the decay coefficient. It is worth noting that they are generated utilizing laboratory data; however, in the current study this relationship is produced by making use of the field data and in addition, its application in a numerical model is verified.

PREVIOUS STUDIES

Many published studies signify the importance and effectiveness of environmental parameters on the FC mortality rate. A number of them, such as Wu et al. (2019), have recognized the relationship between the FC die-off rate and the environmental factors using experimental and laboratory data, and some of them using field data (e.g. Piorkowski et al. 2013; Parkins et al. 2014). However, these types of relationships may not be suitable for numerical models; moreover, having a variable and dynamic FC decay rate for modelling this pathogen is more applicable for future planning and design.

Chamberlin & Mitchella (1978) showed that the decay coefficient is inversely proportional to light, salinity, and heavy metal concentrations. Also, they proposed an equation describing the relationship of the FC decay coefficient and the light intensity. Bitton (1980) reported that temperature is the most important environmental solitary parameter that affects the FC mortality rate, especially in fresh and dark water. Knott’s (1982) studies showed that the mortality rate of coliforms increased when wastewater containing low oxygen entered into the sea with a higher oxygen concentration, and concluded that this phenomenon could be due to the sudden oxygen shock. The studies of Gannon et al. (1985) in Ford Lake in Michigan regarding the effect of daytime and sediment on the FC concentration and its mortality rate illustrated that the sediment concentration plays a crucial role in the overall FC disappearance in the upper end of the lake. An average value of daytime FC decay coefficient of 0.4 h⁻¹ during dry weather was also reported in this study. The effect of sunlight intensity on the coliform die-off rate was investigated by Sarikaya & Saatci (1987). In another survey, the effect of pond depth and sunlight on mortality rate was studied by Mayo & Gondwe (1989). Curtis et al. (1992) investigated the effect of sunlight, dissolved oxygen, and pH on the mortality rate of FC utilizing empirical and theoretical models. They found that light can only have an impact on FC if complemented by high dissolved oxygen (DO) concentrations and a high value of pH. Mayo (1995) modelled the importance of environmental parameters such as sunlight intensity, pond depth, and pH using pilot-scale and full-scale wastewater stabilization ponds. The mortality rate declines with an increasing average pond depth and decreasing sunlight intensity. In this paper, it was also claimed that dissolved oxygen and pH did not have a significant effect on the coliforms die-off rate. Kashefipour et al. (2002) developed an empirical model in which the FC die-off rate was related to sunshine intensity. Garcia-Barcina et al. (2002) investigated the effect of input effluent discharges and weather conditions on the FC concentrations in the Bilbao estuary, located in the north of Spain. This paper implies that in dry weather conditions and suitable operation of effluent outfalls the FC concentration remains within the standard range. Kashefipour et al. (2006) numerically modelled the total and faecal coliforms decay rates using a 2D depth integrated hydro-environmental model which was set up for Irvine estuary in Scotland. In this study, three methods were used to represent the relationship between the decay rate and the level of solar radiation including constant, day- and night-time decay rates, and solar radiation-related time varying decay rate. The outcomes of this study indicated that the accuracy of FC concentration predictions slightly improved when a variable decay rate was used (about 8%). Manache et al. (2007) simulated the FC concentrations in the Chicago Waterway System by assuming
different decay rates for different survey sites, with minimum and maximum values of 0.1 and 1.6 day\(^{-1}\), respectively. Schultz-Fademrecht et al. (2008) examined the effect of sunlight on the decay rate of FC in the laboratory using artificial sunlight. In this study, water and sediment of the Isar River in Germany were used. It was found that the bacteria inactivation mainly depends on the light intensity, for example, the amounts of 21.4, 12.7, and 3.4 day\(^{-1}\) of decay rates were reported for the light intensities of 40, 8, and 0.08 W/m\(^2\), respectively. The effects of wet and dry weathers and sediment concentration on the mortality rate of \textit{Escherichia coli} were also analysed by Wu et al. (2009). Jagupilla et al. (2010) applied a multivariate polynomial regression (MPR) model to determine the nature and magnitude of FC sources in a combined sewer overflow-impacted stretch of the Passaic River in Paterson, New Jersey. This MPR model was used to make the relationship between FC concentrations and some environmental parameters such as temperature, precipitation, discharge, and the entrance FC load coming from upstream. Romeiro et al. (2011) studied the role of longitudinal and transversal diffusion coefficients and the decay rate coefficient on the dynamic modelling of FCs. Huang et al. (2014, 2017) introduced a numerical model to be able to simulate the FC concentration. They evaluated the effect of sediment particles on the fate and transport of faecal organisms and defined some new decay coefficients based on the salinity and sunlight intensity. Gao et al. (2015) developed a model for the fate and transport of faecal bacteria in shallow waters. Also, they evaluated the effects of many processes such as tide, river discharges from upstream, and the amount of FCs entering from boundaries or combined sewer outfalls (CSOs). In this paper, a model was also developed for the decay coefficient as a function of salinity, sunlight intensity and temperature.

**GOVERNING EQUATIONS**

For full scale unsteady non-uniform flow and real time modelling of FCs in river basins, the one dimensional Saint-Venant equations must be numerically solved to specify water elevations and discharges at any time and point. The hydrodynamic continuity and momentum Saint-Venant equations can be written as (Cunge et al. 1980):

\begin{align}
\frac{\partial Q}{\partial x} + T_W \frac{\partial Z}{\partial t} &= q_L \\
\frac{\partial Q}{\partial t} + 2\beta Q q_L \frac{2\beta Q T_W}{A} - 4 \frac{Q^2}{A^2} \frac{\partial A}{\partial x} &= -g A \beta \frac{\partial Z}{\partial x} - \frac{n^2 Q |Q|}{AR^{1.5}}
\end{align}

where \(Q\) (m\(^3\)/s) is discharge; \(A\) (m\(^2\)) is cross section area; \(q_L\) (m\(^2\)/s) is lateral inflow or outflow discharge per unit channel length (positive for inflow and negative for outflow); \(\beta\) stands for momentum correction coefficient; \(T_W\) (m) is top width of water; \(Z\) (m) is water surface elevation; \(g\) (m/s\(^2\)) is gravitational acceleration; \(R\) (m) is hydraulic radius; \(n\) stands for Manning roughness coefficient; \(t\) and \(x\) are time and longitudinal distance in flow direction, respectively.

In any water body such as rivers, the pollutants movement is affected by two main processes including advection and dispersion. Depending on the type of pollutant, the different physical, chemical, and biological processes may affect the concentration of pollutant. FC concentration can be dynamically modelled by the complete form of the dynamic advection-dispersion equation (ADE) which is derived using the mass conservation principle written for FC (Rutherford & O'Sullivan 1974):

\begin{equation}
\frac{\partial S_A}{\partial t} + \frac{\partial S_Q}{\partial x} - \frac{\partial}{\partial x} AD_L \frac{\partial S}{\partial x} = q_L S_L - KSA
\end{equation}

where \(D_L\) (m\(^2\)/s) is the longitudinal dispersion coefficient; \(S_L\) (cfu/100 mL) is the FC concentration for the lateral inflow or outflow; \(S\) (cfu/100 mL) is the FC concentration; and \(K\) (S\(^{-1}\)) is the FC mortality rate or decay coefficient. In many commercial numerical models, the amounts of \(D_L\) and \(K\) are assumed to be constant, however, these two parameters are highly dependent on the hydraulic, channel geometry, and environmental conditions. There are many empirical and/or semi-empirical equations in the literature describing the relationship of \(D_L\) with hydraulic and channel geometry conditions. In this research study, the empirical equation presented by Kashefi & Falconer (2002) is adapted.
The second part of the right-hand side of Equation (3) shows a first-order decay function as
\[ S = S_0 e^{-Kt} \]
where \( S_0 \) is the initial FC concentration at outfall and \( e \) is the Napier number (i.e. 2.7183). Therefore, the relationship between the die-off rate (mortality rate or decay coefficient, \( K \)) and \( T_{90} \) (90% of the coliform bacteria die) is written as
\[ K = \frac{2.303}{T_{90}} \quad (\ln 0.1 = -2.303). \]

**MATERIALS AND METHODS**

In this study, the FASTER model (Flow and Solute Transport model in Estuaries and Rivers), which was initially developed by Kashefipour (2002), was employed to model the FC concentrations and to determine the relationship of decay coefficient with environmental conditions. In the hydrodynamic module of this model, Equations (1) and (2) are numerically solved using an implicit staggered central finite difference scheme with variable grid size, which is unconditionally stable. In the water quality module of this model, Equation (3) is numerically solved utilizing an implicit finite volume scheme. This finite volume-based solution procedure calculates the advection of a concentrate of solute at each face of any control volume by means of a modified form of the highly accurate ULTIMATE QUICKEST scheme. A space staggered grid system is used to solve the finite volume form of the ADE in which the variable \( S \) is located at the centre of the control volume (Falconer et al. 2005).

**Study area**

The FASTER model was setup for a reach of Karun River, the largest and only navigation river in Iran, with the 50 years average discharge of this river being reported to be about 600 m\(^3\)/s. The reach length was 110 km with 113 cross sections. Figure 1 displays the domain study area in which Mollasani (Cross Section 113 or CS-113) and Farsiat (Cross Section 1 or CS-1) are the upstream and downstream boundaries, respectively. From the upstream boundary, the
measured hydrograph, \((Q-t)\), and from the downstream boundary, time-series of water elevations \((Z-t)\), data were given to the model as the boundary conditions to complete the cycle of running program. The measured water elevations and discharges at Ahvaz survey site (Cross Section 49 or CS-49) were used for calibration and verification of the hydrodynamic module of the FASTER model. Also, the measured FC concentrations at CS-113 were used as the upper boundary, and at Zergan (CS-66) were employed for calibration and verification of the water quality module of the model (see Figure 1).

Data source and definitions

During the calibration period for the hydrodynamic module of the FASTER model, three years (2006–2008, simulation time \(\approx 25,000 \text{ h} \)) continuously recorded discharges and water elevations at the hydrometric stations CS-113 and CS-1 were used as the upstream and downstream boundaries, respectively. The measured FC concentrations at the upstream boundary for the same period were utilized for calibrating the water quality module of the FASTER model. Thirty measured FC values were available during this period at all boundaries and the survey sites and were collected from Khuzestan Water and Power Authority (KWPA, www.kwpa.info/en/). These data were also used for the development of the relationship between decay coefficient and environmental parameters. The same data values for the other period, the years 2009–2010 (simulation time \(\approx 9,000 \text{ h} \)) were also available and used to verify the aforementioned developed relationship. For these two periods, the other necessary data including temperature, turbidity, \(pH\) and electrical conductivity \((EC)\) were also available for the sampling times and at the survey sites. The data of wastewater and drainage outfalls (lateral inflows) with their FC concentrations were also available for these two periods. They were defined for the FASTER model through its setup for calibration and verification periods. Table 1 provides a summary of the key survey sites.

| Model module       | U-Boundary | D-Boundary | Calibration period | Verification period |
|--------------------|------------|------------|--------------------|---------------------|
| Hydrodynamic       | CS-113     | CS-1       | CS-49              | CS-49               |
| Water quality      | CS-113     | CS-1       | CS-66              | CS-66               |

(3)). Since bacteria are live creatures, obviously the environmental conditions can change their mortality rates so assuming this coefficient as a constant value during the whole simulation time in a numerical model does not give accurate bacteria predictions. Therefore, the main aim of this study was to develop a relationship between mortality rate or decay coefficient and the environmental parameters such as turbidity, \(pH\), and salinity. During the simulation time, this relationship enables the numerical model to dynamically adjust the amount of decay rate using the measured environmental parameters inserted to the model, resulting in an improvement in the accuracy of the FC concentrations predictions for any desired scenarios. This relationship is produced using the numerical model calibration, and the procedure is described as follows. It was first assumed that the FC decay coefficient \((K)\) is a function of turbidity \((TU)\), temperature \((T)\), \(EC\), and \(pH\):

\[
K = f(TU, T, EC, pH)
\]

During the calibration period, for each measured FC concentration at Zergan survey site (CS-66), a number of model runs were carried out. After each run, the predicted and measured FC values were compared, and before each new run, the initial \(K\) value was manually adjusted. These runs were continued until the predicted and measured FC concentrations at this sampling time were precisely the same or very close together, without considering the other measured FC values at this survey site and for the other sampling times. Thus, a proper \(K\) for an appropriate time \((t)\) is determined (i.e. \(K_1\)). For this time, the other considered environmental parameters from the measured data are also specified \((TU_1, T_1, EC_1, \text{ and } pH_1)\). This procedure was separately carried out for all of the sampling times \((t_1, t_2, t_3, \ldots)\) and the measured FC concentration values \((FC_1, FC_2, FC_3, \ldots)\). Therefore, the appropriate \(K\) values
(\(K_1, K_2, K_3, \ldots\)) were determined with this procedure for all existing sampling times, and the corresponding measured \(TU\), \(T\), \(EC\) and \(pH\) were specified from the measured data. It was therefore possible to correlate the \(K\) values with the corresponding \(TU\), \(T\), \(EC\) and \(pH\) employing the regression analysis to find the best equation describing the relationship of mortality rate with the considered environmental parameters. This equation was then added to the water quality module of the FASTER model as a part of the numerical solution of the ADE. Thus, for the verification period or any desired scenarios, at any time step during the simulation, the model is able first to calculate the proper decay coefficient using the measured environmental parameters and then to complete the whole numerical solution of the ADE.

Model evaluation

After developing the relationship of the decay coefficient of FC with environmental parameters, it is necessary to evaluate the model performance in predicting the FC concentrations. In the current study, the model evaluation was carried out using three statistical factors, including the following. (1) The slope (\(a\)) of a line between the predicted and measured values of a desired variable with an acceptable determination coefficient (\(R^2\)). It is obvious that for a better and more accurate simulation, these two values should be close to unity. This line is defined as:

\[ X_M = aX_P \]  

(5)

(2) Average absolute error which is defined as:

\[ E = \frac{\sum |X_M - X_P|}{\sum X_M} \times 100\% \]  

(6)

(3) Root mean square error which is defined as:

\[ RMSE = \left[ \frac{\sum_{i=1}^{N} (X_M - X_P)^2}{N} \right]^{0.5} \]  

(7)

where \(X\) stands for FC concentration, and \(M\) and \(P\) are two subscripts indicating the measured and predicted FC, respectively; \(N\) is the number of data.

RESULTS AND DISCUSSION

Calibration and verification of hydrodynamic module

In water quality modelling, first it is necessary to calibrate and verify the hydrodynamic module of the numerical model to make sure that during the whole simulation time, water elevations and discharges are accurately modelled. As mentioned previously, the measured water elevations and discharges at Ahvaz hydrometric station (CS-49 in Figure 1) were used for calibration and verification periods. Calibration and verification of the hydrodynamic module of the FASTER model employing the dynamic and variable Manning roughness coefficient as a function of discharge, flow depth and velocity for these two periods are fully described in Mohammadi & Kashefipour (2014).

Calibration and verification of water quality module

As previously mentioned, the model calibration procedure was used to develop an empirical relationship between decay coefficient (\(K\)) and environmental parameters. After specifying the decay coefficient values (\(K_1, K_2, K_3, \ldots\)) using the model calibration and the corresponding environmental parameters (\(TU_1, T_1, EC_1, pH_1, TU_2, T_2, EC_2, pH_2, \ldots\)) from the measured data, the nonlinear multivariable regression analysis was applied to produce this relationship. The best equation was obtained as:

\[ K = 0.012I + 0.01I^2 + 0.009J + 0.004J^2 - 0.021I + 0.014R^2 \]

where \(TU\) is turbidity (NTU or Nephelometric Turbidity Units); \(T\) is temperature (°C); \(K\) is decay coefficient (h\(^{-1}\)); \(I = \ln (TU)\); \(J = \ln (T)\).

It was found that pH is not a significant parameter affecting the FC concentration. This could be due to a narrow range of pH variations along the considered periods (7.5–8.4). However, many researchers reported that either pH is not an important parameter (Mayo 1995) or is conditionally effective (Curtis et al. 1992). Since the EC values
were in a small range (mostly around 1,750 ds/m, with the maximum and minimum values of 1,250 and 3,070 ds/m, respectively), no appropriate relationship was found between the mortality rate and this environmental parameter. Equation (8) was then included in the water quality module of the numerical FASTER model. Therefore, during each time step for the verification period or any scenarios and any new simulations, the decay coefficient ($K$) was first dynamically calculated utilizing this empirical equation and the measured turbidity and temperatures and Equation (3) was then numerically solved to predict the FC concentrations for all nodes along the simulation domain. The performance of Equation (8) in improving the model accuracy during calibration mode is illustrated in Table 2. In this table, the comparative statistical parameters for the predicted and measured FC concentrations were calculated. A constant but best value for decay coefficient ($K = 0.05$ h$^{-1}$) was also specified after several runs of the model, and the comparison of the measured and predicted FC concentrations during the calibration period are also shown in the table. Table 2 shows that the variable decay coefficient generally performs better than the constant one for modeling FC bacteria. Comparison of the predicted and measured FC concentrations when the variable decay coefficient is calculated using Equation (8) during the calibration period is also shown in Figure 2. In this figure, the predicted FC concentrations when $K = 0.05$ h$^{-1}$ are also compared with the corresponding measured values. The maximum and minimum decay coefficients during the calibration period were estimated using Equation (8) equal to 0.341 and 0.006 h$^{-1}$, respectively. The corresponding values for the verification period were calculated as 0.155 and 0.004 h$^{-1}$. The average decay coefficients for calibration and verification periods were calculated as 0.024 and 0.52 h$^{-1}$, respectively.

The predicted and measured FC concentrations during the verification period are compared in Figure 3 for both the variable (Equation (8)) and the constant decay coefficient ($K = 0.05$ h$^{-1}$). The calculated statistical parameters for this period are depicted in Table 3. As can be seen from this table, the accuracy of the model was improved for the variable and dynamic FC decay coefficient.

**DISCUSSION**

The data used in this study were provided from a water agency and those data are commonly measured at the

| $K$ (h$^{-1}$) | $a$ | $R^2$ | $E$ (%) | RMSE (cfu/100 mL) |
|---------------|-----|-------|---------|-------------------|
| Equation (8)  | 0.96| 0.87  | 28.60   | 2,706             |
| 0.05          | 0.72| 0.93  | 51.40   | 5,353             |
hydrometric stations along Karun River, southwest Iran. These types of data are usually measured at hydrometric
stations around the world, so with the procedure described in this study it would be possible to correlate the FC decay coefficient to the environmental parameters (variable \( K \)), and easily model the FC concentration can be easily modelled more precisely than using a constant decay coefficient. Therefore, producing the relationship as mentioned above utilizing the real and field data is realistic, and any laboratory undesirable effects such as scale effect is ignored since scale is effective in the dispersion and advection processes of pollutants.

In this study, four quality parameters were considered to generate an equation for describing and calculating the FC mortality rate using environmental conditions. Although it is proved by many scientists that salinity and acidity are two key parameters for FC bacteria population, it was found that there is no clear relationship between these two parameters and FC mortality rate. This could be due to the existing low range of both quality parameters, hence the generated equation did not show any sensitivity to these parameters. Two other quality parameters were turbidity and temperature, with the effect of turbidity being more than temperature (see Equation (8)). Turbidity in rivers is generally the consequence of existing fine sediment in suspended form. Increasing turbidity means higher sediment concentration, which itself is effective on the fixation, fate, and transport of FC bacteria. Another effect of this parameter is light penetration which is reduced with increasing turbidity, which may reduce the mortality rate of FC. The main point is that turbidity shows the combination effect of suspended sediment concentration and light intensity. Previous studies have shown that light intensity seriously affects the bacterial mortality rate. It is better to separately investigate the effects of suspended sediment concentration on the fate and transport of faecal bacterial indicator.

**CONCLUSIONS**

In this study, a new empirical equation was developed utilizing numerical model calibration (one-dimensional FASTER model) in which the decay coefficient or mortality rate was related to the water temperature and turbidity for numerically modelling of FC indicators. This equation was then added to the water quality module of the FASTER model. During each time step of the simulation time, this key coefficient is first estimated by using this equation, and its amount
is then used for completing the numerical solution of the Advection-Dispersion Equation (ADE). All measured necessary data were available for Karun river, southwest Iran, and the model was set-up for two different periods, including the years of 2006–2008 (model calibration) and 2009–2010 (model verification). It was found that water temperature and turbidity are the key environmental parameters affecting the mortality rate of faecal bacteria, and pH is not prominent among the considered parameters since its variation range was low (7.5–8.4). Also, for a similar reason, EC did not show a good relationship with the mortality rate. A comparison of the predicted and measured FC concentrations shows that applying a dynamic and variable decay coefficient instead of a constant value remarkably increased the model accuracy (about 23 and 20% for calibration and verification periods, respectively). Finally, the accurate estimate of faecal bacterial concentration is generally a function of aquatic environmental parameters. Of course, many other parameters such as suspended sediment concentration may be important in the FC concentration due to settling with particles or vice versa, and more research is needed to correlate these parameters together.

ACKNOWLEDGEMENTS

The authors are grateful to the Khuzestan Water and Power Authorities (KWPA) for provision of the data, and they are also grateful for the funding provided by Vice-Chancellor’s Office for Research Affairs of Shahid Chamran University of Ahvaz.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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First received 26 April 2020; accepted in revised form 17 July 2020. Available online 19 August 2020