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Andrew R. Slaughter

Institute for Water Research, Rhodes University, a.slaughter@ru.ac.za

Sukhmani K. Mantel

Institute for Water Research, Rhodes University, s.mantel@ru.ac.za

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Modelling microbial water quality across multiple temporal scales

Andrew R. Slaughter¹, Sukhmani K. Mantel²

Institute for Water Research, Rhodes University, Grahamstown, South Africa [1a.slaughter@ru.ac.za](mailto:a.slaughter@ru.ac.za);
[2s.mantel@ru.ac.za](mailto:s.mantel@ru.ac.za)

Abstract: Microbial water quality can have profound effects on human health. Microbial water quality modelling can be a useful tool for water quality management in catchments. Since flow drives water quality, water quality models rely on estimates of flow from hydrological and systems models. However, these different hydrological and systems models operate over different time steps, which may be mismatched to those of flow processes affecting microbial water quality. Therefore, the aim of this study was to investigate the accuracy of microbial water quality modelling across different time steps, thereby assessing which flow time steps are suitable for driving microbial water quality modelling. *Escherichia coli* was modelled as an indicator of microbial water quality. For monthly modelling, the Water Evaluation and Planning Model (WEAP) was applied to the upper catchment of the Crocodile River in Mpumalanga, South Africa. For the above application, *E. coli* was modelled in WEAP using first-order degradation. For daily modelling, monthly flows from the upper Crocodile River were disaggregated to daily and modelled using the Water Quality Systems Assessment Model (WQSAM). Model simulations were assessed against available observed data. WQSAM managed to represent the full variability of the observed data at a daily time step. This was not the case for WEAP at a monthly time step. The results indicate that for integration of water management and water quality models for microbial water quality modelling, integration will have to take place at a daily or sub-daily time step.

Keywords: Microbial water quality; water quality modelling; temporal scales

1 INTRODUCTION

Poor microbial water quality remains a challenge for many countries. Whereas developed countries are increasingly focussing on non-point sources of microbial contaminants (Wilkinson et al., 2006), developing countries continue to struggle to manage both point- and non-point sources of contaminants. A good example is South Africa, where waste water treatment plants (WWTPs) are inadequately managed and are often overloaded (Britz and Sigge, 2012). Microbial contamination of water occurs mainly through faecal contamination, which results in the input of a wide range of pathogens such as bacteria, protozoans and viruses. Since testing for a wide range of microbial pathogens is prohibitively expensive and complex, faecal indicator species are typically tested for, which can act as a general indicator of the degree of faecal contamination of water. The indicator species is typically relatively cheaply and easily measured and may be relatively harmless, but can provide a model of the loading and instream concentrations of other pathogens introduced through faecal contamination (Hipsey et al. 2008). Most commonly, the indicator species are Gram-negative enteric coliform bacteria of the family Enterobacteriaceae (Hipsey et al., 2008), such as total coliforms, faecal coliforms and *Escherichia coli*. *E. coli* has been suggested to be the most appropriate faecal indicator species by recent studies (Edberg et al., 2000; USEPA, 2001; Sokolova et al., 2013), although this is not without criticism as studies have shown different classes of organisms show a wide range of responses to environmental pressures (Hipsey et al., 2008).

The modelling of microbial water quality can assist in the management of water resources, particularly within a context of increasing water insecurity due to increasing development and climate change.

Although our knowledge of the behaviour of microorganisms at the ecosystem level remains incomplete (Venter et al., 2011), microbial water quality modelling can guide in the prioritisation of mitigation measures by indicating individual sources of contamination (Sokolova et al., 2013).

Water resources management models allow the equitable sharing of water among multiple water users, particularly under water-stressed conditions, and also the investigation of the impacts of different management scenarios of water availability. Since water quantity is a driver of water quality, water quality models should integrate with water resources management models for the implementation of Integrated Water Resources Management (IWRM). For example, investigating management scenarios in a water resources management model, such as increasing the capacity of a WWTP, would have a dramatic effect on water quality.

Traditionally, water resources management models have been operated at time steps ranging from yearly to weekly, as these time steps have been regarded as adequate for the needs of water quantity management. For example, the Water Resources Yield Model (WRYM) (Basson et al., 1994), routinely operated in South Africa, is operated at a monthly time step. However, water quality processes that would typically affect microbial water quality, such as rainfall-runoff and water temperature, may operate at daily or sub-daily time steps. This poses a barrier to integration of water quality models with water resources models. Daily-time-step water resources modelling is not often attempted because models of such a fine temporal resolution are generally not required for water quantity management and it would be a data- and resource-intensive exercise, particularly since these models are typically used for long-term planning and may be run for simulations of tens of years. The Water Quality Systems Assessment Model (Slaughter et al., 2017) uses a monthly-to-daily flow disaggregation technique (Slaughter et al., 2015) to overcome this problem, thereby allowing a daily-time-step water quality model to be integrated with a monthly-time-step water resources model.

Knowledge on appropriate time steps required to model microbial water quality can assist in the integration of microbial water quality modelling with water resources management modelling. This study therefore aims to assess the suitability of two time steps of modelling microbial water quality within water resources management modelling, namely monthly and daily.

2 METHODS AND STUDY AREA

2.1 Study area

The Crocodile River catchment, which is situated in the province of Mpumalanga in the north-east of South Africa (Figure 1), has its source in the Highveld and drains an area of 10,440 km² over a total distance of 320 km, although the present study modelled *E. coli* within the upper reaches of the catchment as most observed data is concentrated in this region. Rainfall in the catchment decreases from west to east, ranging from 600 mm–1,200 mm with a mean of 880 mm, and a seasonal rainfall with a summer maximum (Deksissa et al. 2004). The catchment is of economic importance and water is exploited for extensive agriculture, which is mostly wheat and maize farming in the upper catchment. Point sources of industrial and domestic origin also introduce pollution into the river.

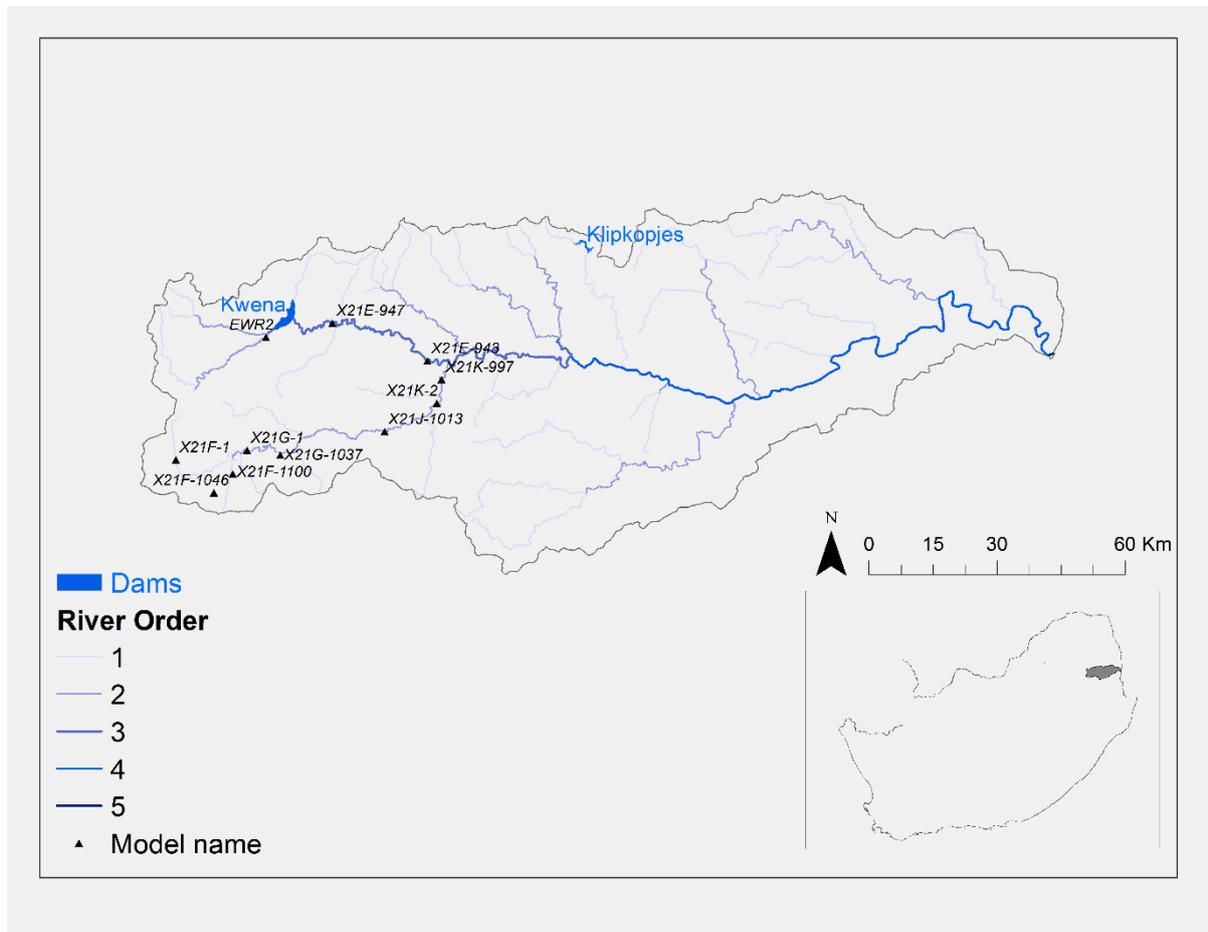


Figure 1. Location of monitoring points within the Crocodile River catchment containing observed data for *Escherichia coli*

2.2 Observed data

The monitoring points containing data for *E. coli* are indicated in Figure 1. Table 1 provides a statistical summary of the observed data used in the study for the two monitoring points.

2.2 Modelling procedure

The Water Evaluation and Planning (WEAP) model was developed by the Stockholm Environment Institute, and uses the basic principle of water balance as a tool for water resources planning and management (Psomas *et al.*, 2016). The model is able to represent a wide range of water system elements and water allocation policies. WEAP includes basic water quality modelling functionality. *E. coli* was added as a non-conservative water quality variable in WEAP. WEAP models a non-conservative water quality variable through first-order degradation, where a single degradation rate is applied throughout the entire modelled catchment. Concentration values for *E. coli* were assigned to subcatchment water inflow in WEAP, and the global degradation rate was adjusted as a calibration exercise to visually fit as closely as possible the simulated data to the available observed data.

The Water Quality Systems Assessment Model (WQSAM) (Slaughter *et al.*, 2017) is a daily-time-step water quality model that was developed specifically to integrate with routinely-used water resources management models in South Africa. Microbial water quality modelling capacity has been added to WQSAM (Slaughter, 2017). WQSAM subscribes to a requisite simplicity approach to modelling water quality, representing only the processes that explain the majority of variation in observed water quality data. In this way, WQSAM aims to remain a relatively simple water quality model, thereby limiting the amount of observed data required for calibration.

Table 1 List of monitoring points within the middle Crocodile River Catchment, Mpumalanga, South Africa containing observed *Escherichia coli* data as cells 100 mL⁻¹ that were used in this study

Model Node Name	Coordinates		n	Dates		cells 100 mL ⁻¹			SD
	Lat.	Lon.		from	to	mean	min.	max.	
EWR2	-25.40	30.33	46	2008	2012	307.78	0.00	1,732.00	469.24
X21F_1100*	-25.69	30.26	132	2004	2012	561.24	0.00	12,100.00	1,149.89
X21F_1100*	-25.72	30.24	28	2008	2010	128.33	0.00	1,300.00	311.13
Waste Water Treatment Plant (WWTP) data									
X21F-1100*	-25.69	30.25	31	2008	2011	241.17	0.00	2,419.00	643.76

* These are three separate datasets of observed data collected in the same modelled region

The WQSAM representation of *E. coli* is slightly more sophisticated than that of WEAP, following the procedure of Sokolova et al. (2013). Within this formulation, although degradation is also regarded as a first-order rate, salinity and water temperature mediate the degradation rate, and therefore also need to be simulated. WQSAM also allows for the setting of degradation rates for individual subcatchments, allowing more flexibility for representation of different process rates across a modelled catchment.

Since WEAP is not able to simulate water quality for reservoirs, the comparisons between models were made for two stations upstream of reservoirs, namely EWR2 and X21F-1100.

3 RESULTS

3.1 Results for WEAP

A high degradation rate of 0.9 d⁻¹ was used in WEAP for *E. coli* modelling. To simulate the input of *E. coli* at the X21F headwater, monthly concentrations were used, with a high of 12,000 cells 100 mL⁻¹ during summer and a low of 100 cells 100 mL⁻¹ during winter, to represent higher runoff during summer in this summer rainfall region. For the waste water return flow within the X21F catchment, the Random Distribution function in WEAP was used with a mean of 300 cells 100 mL⁻¹ and a standard deviation of 100 cells 100 mL⁻¹. This is because it has been found that waste water treatment works (WWTWs) in South Africa release effluent of highly variable flow and water quality that can be represented by a random distribution (Slaughter and Hughes, 2013). This has been attributed to WWTWs being overloaded and inefficiently managed. For the headwaters above the point EWR2, monthly concentrations were used, with a high of 2,000 cells 100 mL⁻¹ during summer and a low of 100 cells 100 mL⁻¹ during winter.

The WEAP model could not represent the full variability of the observed *E. coli* data, as can be seen in Figure 2. For the X21F-1100 point, the Nash Sutcliffe Efficiency (Nash and Sutcliffe, 1970) (NSE) obtained was very bad at -3.92 (Figure 2a). The NSE obtained for EWR2 was also not good at -2.92 (Figure 2b).

3.2 Results for WQSAM

Within WQSAM, temperature and salinity are used within the equation to simulate *E. coli* survival. For the most part, WQSAM gave reasonable estimates of water temperature and salinity (Slaughter, 2017). Model simulations of *E. coli* were relatively good, with the model generally representing a large majority of the variation in the observed *E. coli* data. The NSE obtained for X21F-1100 was 0.60 (Figure 2a) and the NSE obtained for EWR2 was 0.97 (Figure 2b).

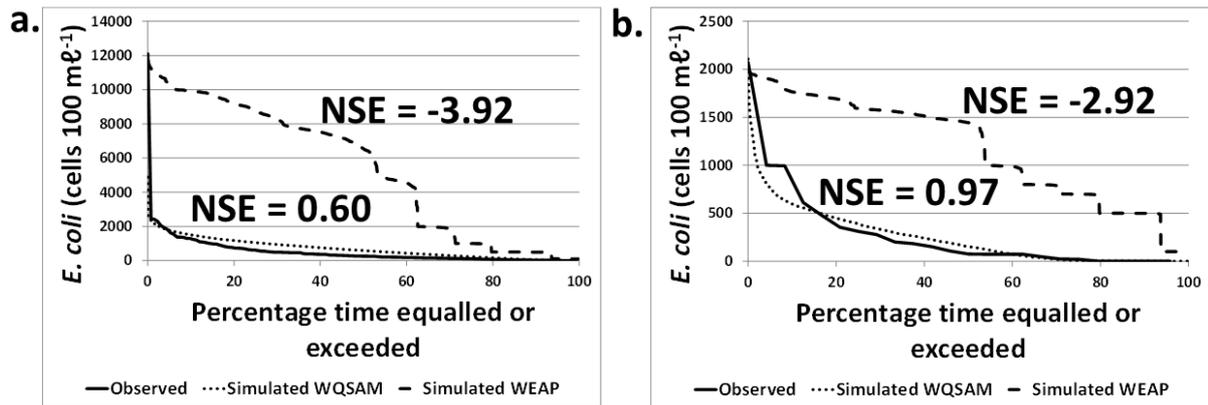


Figure 2. Results of simulations of *Escherichia coli* within the Water Evaluation and Planning (WEAP) model and the Water Quality Systems Assessment Model (WQSAM) compared to observed data as frequency distributions for X21F-1100 (a) and EWR2 (b).

4 DISCUSSION

WQSAM managed to represent the vast majority of the variation in observed *E. coli* data for the two monitoring points. However, even at a daily time step, WQSAM struggled to simulate the full frequency distribution of observed data (Figure 2a). WEAP could not represent the full variability of observed *E. coli* data at a monthly time step (Figure 2a and 2b). This indicates that for integration of water quality and water resources management models for modelling non-conservative water quality variables such as microbial water quality, a daily or sub-daily time step is required in the integration. Most water resources management models routinely used in management are run on weekly, monthly or yearly time steps, for example, the WRYM in South Africa and the CALSIM model in California are both run on monthly time steps. Integration with daily-time-step water quality models can be achieved with these monthly-time-step water resources management models in two ways: either the water resources management models can be updated to run on a daily time step, or as in the case of WQSAM, a monthly-daily flow disaggregation procedure (Slaughter et al., 2015) can be used. The design and implementation of daily-time-step water resources management models are fraught with uncertainties and challenges, as for the most part, these models have not been established, and would require large datasets, computer resources and time to run. The monthly-daily flow disaggregation procedure, although associated with some uncertainties, provides an easy and low-data, low resource method to achieve daily flow data from a monthly water resources management model.

It must be considered that water quality simulation capacity offered in WEAP is very simple and would not provide a very good representation of complex water quality processes, particularly for non-conservative water quality variables such as microbial water quality. For example, the degradation coefficient in WEAP is applied globally, i.e., you cannot set this for individual subcatchments in the model. WEAP also uses a generic first-order degradation equation for non-conservative water quality variables, when a more realistic process description for *E. coli* fate should also consider temperature and salinity (Sokolova et al., 2013).

A limitation of this study was the small number of monitoring points compared between the models. This approach was taken because WEAP cannot model water quality in reservoirs, and the two monitoring points chosen are above reservoirs in the catchment. This is an initial study, and extensive improvement could be achieved through extension to consider further data and monitoring points in the catchment.

5 CONCLUSIONS AND RECOMMENDATIONS

Modelling of non-conservative water quality variables such as microbial water quality needs to be done at a time step of daily or finer to sufficiently represent the most important water quality processes. In contrast, water resources management models are often run at a monthly time step. In terms of time step, a viable compromise needs to be found for the integration of water resources management models

and water quality models. Modelling at a daily time step appears to be of sufficient resolution to model non-conservative water quality variables such as *E. coli*. Therefore, the integration of water quality models and water resources management models should be done at a temporal resolution of daily or finer for modelling non-conservative water quality variables such as microbial water quality. Integration could be achieved by either the implementation of a daily-time-step water resources management model, which faces many challenges, or through a monthly-daily flow disaggregation procedure, such as is implemented in WQSAM.

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