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Development and evaluation of the bacterial fate and transport module for the Agricultural Policy/Environmental eXtender (APEX) model

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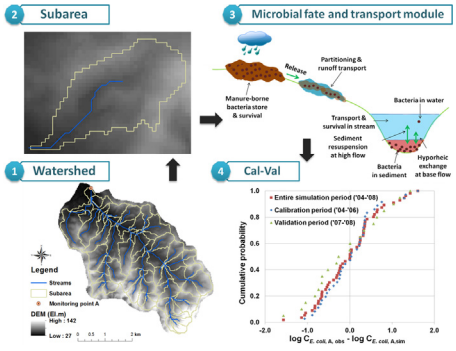
HIGHLIGHTS

- The APEX model can benefit from addition of a bacteria fate and transport module.
- APEX manure erosion submodel drives manure bacteria release and export.
- The two-stage kinetics and thermal time to simulate fate of bacteria in manure deposits.
- Sediment resuspension and hyporheic exchange provide the in-stream bacteria source.
- Successful performance was found with *E. coli* monitoring data at the Toenepi watershed.

GRAPHICAL ABSTRACT



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ABSTRACT

The Agricultural Policy/Environmental eXtender (APEX) is a watershed-scale water quality model that includes detailed representation of agricultural management. The objective of this work was to develop a process-based model for simulating the fate and transport of manure-borne bacteria on land and in streams with the APEX model. The bacteria model utilizes manure erosion rates to estimate the amount of edge-of-field bacteria export. Bacteria survival in manure is simulated as a two-stage process separately for each manure application event. In-stream microbial fate and transport processes include bacteria release from streambeds due to sediment resuspension during high flow events, active release from the streambed sediment during low flow periods, bacteria settling with sediment, and survival. Default parameter values were selected from published databases and evaluated based on field observations. The APEX model with the newly developed microbial fate and transport module was applied to simulate fate and transport of the fecal indicator bacterium *Escherichia coli* in the Toenepi watershed, New Zealand that was monitored for seven years. The stream network of the watershed ran through grazing lands with daily bovine waste deposition. Results show that the APEX with the bacteria module reproduced well the monitored pattern of *E. coli* concentrations at the watershed outlet. The APEX with the microbial fate and transport module will be utilized for predicting microbial quality of water as affected by various agricultural practices, evaluating monitoring protocols, and supporting the selection of management practices based on regulations that rely on fecal indicator bacteria concentrations.

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1. Introduction

Every year approximately 76 million people in the U.S. experience foodborne diseases (Painter et al., 2013). Fresh produce is recognized as a source of foodborne disease outbreaks not only in the U.S. but also in many regions of the world (Anderson et al., 2011; Painter et al., 2013; Ceuppens et al., 2014; Hong et al., 2017). Pathogenic microorganisms in irrigation and recreational waters have remained the subject of concern. These pathogens originate primarily from animal waste and wastewater (Liu et al., 2013; Strawn et al., 2013; Holvoet et al., 2014; Hruby et al., 2016).

Water quality models can be essential tools for alleviating pathogen load to water sources, evaluating microbial contamination-related risks, guiding the microbial water quality monitoring, and assessing the effect of agricultural management on the microbial water quality (Parajuli et al., 2009; McBride and Chapra, 2011; Kay et al., 2012). Several models have been developed and evaluated for microbial water quality diagnostics, monitoring, prediction and management (Cho et al., 2016). The Soil and Water Assessment Tool (SWAT) microbe module was developed by (Sadeghi and Arnold, 2002) and applied for simulating fate and transport of fecal coliforms for total maximum daily loads (Benham et al., 2006). The Watershed Analysis Risk Management Framework (WARMF) model was applied to assess suspended sediment and bacterial loadings, depending on various land uses and sources (Joe et al., 2009). A bacteria water quality model was developed and added to Watershed Assessment Model (WAM) to simulate fecal indicator bacteria (Collins and Rutherford, 2004). The Enhanced Stream Water Quality (QUAL2E) model (Gautam et al., 2006), the Water Quality Analysis Simulation Program (WASP5) and the Stormwater Management Model (SWMM) were applied to determine Total Maximum Daily Loads (TMDLs) for fecal coliforms released from an urban watershed (EPA-Region4, 2000).

Models of microorganism fate and transport are often added to existing watershed-scale water quality models; however, specific processes in water quality models can create limitations for microbial modeling. For example, SWMM only addresses urban watersheds by simplistically considering build-up and wash-off to simulate fate and transport of microorganisms. The relatively coarse representation of agricultural practices in the majority of watershed-scale models may be why no explanatory model of interregional differences and intraregional variations in microbial quality of irrigation water has been proposed to date (Pachepsky and Shelton, 2011).

The Agricultural Policy/Environmental eXtender (APEX) is the watershed-scale water quality model that includes highly detailed representation of agricultural management such as irrigation, tillage operation, conservation practices and cropping system as well as surface runoff and losses of sediment and manure (Williams and Izaurralde, 2006). APEX currently does not have microbial fate and transport simulation capabilities. If the microbial fate and transport submodel is developed for the current APEX model, it can be a useful tool to investigate the site-specific potential for microbial contamination and develop management practices for making decision and regulations.

The objective of this work was to develop the first APEX bacterial fate and transport module that could use the APEX model of watershed processes, current knowledge about the microbial fate dynamics, and recently introduced concepts of the in-stream microbial fate and transport.

2. Bacterial fate and transport module development

2.1. The overview of the APEX model

The APEX model is a distributed, continuous, farm- or small watershed-scale hydrologic and water quality model. It is an extension of the Environmental Policy Integrated Climate (EPIC) model. Many of the algorithm development for field-level processes have occurred in EPIC first and then were translated to APEX (Williams et al., 2012). The model is capable of detailed field scale modeling, routing, and thus connecting farm/field sized subareas within a watershed (Tuppad et al., 2009; Wang et al., 2011a). APEX works with a daily time step and can perform long-term simulations to assess impacts of different farm management and conservation practices, and other management activities on surface runoff and losses of sediment, nutrient, and other pollutant indicators (Srivastava et al., 2007; Gassman et al., 2010). The APEX model consists of 12 major components: climate, hydrology, crop growth, pesticide fate, nutrient cycling, erosion-sedimentation, carbon cycling, management practices, soil temperature, plant environment control, economic budgets, and subarea/channel routing. Management practices include: irrigation, fertilizer application, manure management, crop rotation and selection, cover crops, biomass removal, grazing, and tillage. A watershed in APEX is divided into subareas. Subarea are assumed to be homogeneous, i.e. the same crop or land use, weather, soils, topography, and land management. Subareas are spatially related to one another: the entire area within a subarea supplies flows to another subarea inlet. The routing scheme simulates interactions between subarea involving surface runoff, return flow, sediment deposition and degradation, nutrient transport, groundwater flow and analysis for all subareas (Wang et al., 2011b).

2.2. Structure of the bacterial fate and transport module

Simulations can be done for a single strain or a group of fecally-derived bacteria that can be enumerated in manure, animal waste, soil, stream bottom sediment, and water. Below both animal manure and deposited animal waste are called manure for the sake of brevity. The bacterial fate and transport module considers release with manure material due to manure erosion, survival and die-off of bacteria, transport in runoff, and in-stream processes. The module utilizes manure erosion rates, runoff, infiltration, the amount of suspended sediment and streamflow found in the APEX. The main source of the bacteria is applied manure that is released in suspension to runoff and partially transported to deep soil layers. The total number of removed bacteria is found from the concentrations of bacteria in manure and eroded manure amount. Bacteria survival in manure is simulated with the two-stage thermal time-dependent survival model. Survival patterns are simulated separately for each manure application date. Simulated in-stream microbial fate and transport processes include the reach-scale release of bacteria with resuspended streambed sediment during high flow events, the release of bacteria from streambed sediment due to the hypothetic exchange, the deposition with settling sediment, and the thermal time-dependent survival.

2.3. Algorithms of the microbial fate and transport module

The algorithms below are given for the specific strain or group of bacteria of interest that are simulated. For example, “bacteria” below may mean fecal indicator organisms, *Escherichia coli*, enterococci, thermotolerant coliforms, total coliforms, etc.

2.3.1. Manure application, animal waste deposition, and survival

The increase of the total number of microorganisms after manure application or animal waste deposition is computed as.

$$N_d = M_a \cdot N_i \quad (1)$$

$$N_m^+ = N_m + N_d \quad (2)$$

where N_d is the total number of deposited bacteria in daily manure application (CFU ha^{-1}), M_a is the amount of applied manure or waste (MT of manure ha^{-1}), here and below MT stands for metric ton, N_i is the initial number of bacteria in manure (CFU (MT of manure)$^{-1}$), N_m^+ is the daily increase in the total number of bacteria due to deposition

(CFU ha^{-1}), and N_m is the total number of bacteria in animal waste or manure above ground at the beginning of the day (CFU ha^{-1}).

Manure erosion may occur upon runoff events. Applied manure is subject to weathering and bioturbation between rainfall events. If manure is plowed in, the initial value of bacteria on manure is obtained by distributing bacteria from the incorporated manure across the plow layer and then by considering only bacteria in the top one centimeter-thick soil layer. The fate and transport of manure-borne bacteria is simulated on daily basis as shown in equation:

$$\begin{aligned}\Delta N_m &= \text{Deposition–inactivation–export in runoff} + \text{regrowth}\\ &= N_d - \left(10^{-k_s}\cdot N_m^+\right) - \left(\frac{M_e}{M_t}\cdot N_m^+\right) + \left(10^{k_r}\cdot N_m^+\right)\end{aligned} \quad (3)$$

where ΔN_m is the daily change of total number of bacteria in manure (CFU ha^{-1}), k_s is the rate of fecal indicator organism inactivation in manure which is a function of the thermal time and manure properties (day^{-1}), M_e is the amount of eroded manure (MT ha^{-1}), M_t is the total manure amount present on that date (MT ha^{-1}), and k_r is a constant value added to the logarithm of concentration due to regrowth of fecal indicator organism caused by rainfall.

The manure erosion is estimated in APEX as:

$$M_e = k_e\cdot\left(Q\cdot q_p\right)^{0.5}\cdot PE\cdot SL\cdot M_t^{p_1}\cdot e^{-p_2\cdot AGPM} \quad (4)$$

where k_e is the erosion rate coefficient, Q is the daily runoff (mm), q_p is the peak runoff rate (mm h^{-1}), PE is the erosion control practice factor, SL is the slope length and steepness factor, $AGPM$ is the standing live and dead plant material (T ha^{-1}), and p_1 and p_2 are parameters reflecting the sensitivity of M_e to the total amount of manure and aboveground biomass.

Bacteria survival in manure depends on the type of manure, temperature, time after application, and incorporation (Park et al., 2016). Bacteria survival in manure or animal waste is simulated with a two-stage log-linear equation. The rate constants are dependent on temperature that controls bacteria survival (Franz et al., 2008a; Martinez et al., 2013; Park et al., 2016). The daily change in the decimal logarithm of total number of bacteria is simulated as:

$$logN = -k_{s,m} \quad (5)$$

$$k_{s,m} = \begin{cases} k_{s,1,m}(T), & t \le t_{s,m,1} \\ k_{s,2,m}(T), & t > t_{s,m,1} \end{cases} \quad (6)$$

where $k_{s,m}$ is the rate coefficient which is the function of temperature at time t, $t_{s,m,1}$ is the duration of the first stage (day), T is the average daily temperature (°C), and $k_{s,1,m}(T)$ and $k_{s,2,m}(T)$ are survival rates at the first and second survival stage respectively.

The bacteria population may grow, remain stable or die off during the first survival stage, and definitely decrease during the second stage of survival. At the second stage, the values of $k_{s,2}(T)$ can be described with the Q_{10} model (Martinez et al., 2013).

$$k_{s,2,m}(T) = k_{s,2,m}(20)Q_{10,m}^{\frac{T-20}{10}} \quad (7)$$

where $k_{s,2,m}(20)$ is the survival rate at 20 °C, $Q_{10,m}$ reflects the sensitivity of $k_{s,2,m}$ to temperature that is equal to the change in survival rate occurring as temperature changes by 10 °C. Increase in temperature causes increase in the value of $k_{s,2,m}$ and faster inactivation.

The new bacteria submodel assumes growth on a rainy day. According to Martinez et al. (2013), periods with sudden increases in *E. coli* concentration corresponded with rainfall. The effect of several sequential rainy days to bacteria growth is not known and therefore only the first rainy day is assumed to promote the growth with the rate k_r (see Eq. (3)). Bacteria export in runoff depends on the amount of eroded manure. The fraction of bacteria exported with eroded manure is assumed proportional to the fraction of manure that is exported. The manure erosion equation is further modified to account for manure weathering.

$$k_e = p_3\cdot 10^{-k_w\cdot t_a} \quad (8)$$

where p_3 is manure erosion equation coefficient, k_w is the manure weathering rate coefficient (day^{-1}), and t_a is the manure weathering time, i.e. time between manure application and rainfall (day).

Fate and transport of bacteria from each manure application are simulated separately for manure deposited on different days. Manure erosion and bacteria export is simulated proportionally to the fraction of the remaining manure from application the application day in the total amount of manure available to date.

2.3.2. In-stream bacterial fate and transport processes

In-stream microbial fate and transport processes are simulated at the reach scale and include 1) passive release of bacteria with resuspended streambed sediment during high flow events, 2) the transport of bacteria from streambed sediment during low flow periods, 3) the deposition with settling sediment, and 4) die-off and survival.

Sediment is routed through the channel in APEX. The sediment routing equation is a variation of Bagnold's sediment transport equation (Bagnold, 1977; Williams et al., 2012). The transport concentration capacity as a function of velocity is calculated as follows:

$$CY_U = CY_1\cdot v_{ch}{}^{p18} \quad (9)$$

where CY_U is the potential sediment concentration in MT m^{-3} for the flow velocity v_{ch}, CY_1 is the potential sediment concentration for velocity equal to 1.0 m s^{-1}, and $p18$ is a parameter set at 1.5 in Bagnold's equation.

The potential change in sediment yield through a routing reach is calculated as follows:

$$YU = 10\cdot QCH\cdot(CY_U - CIN) \quad (10)$$

where YU is the potential change in sediment yield (MT ha^{-1}), QCH is the volume of flow through the channel (mm), CIN is the inflow sediment concentration (MT m^{-3}), YU is deposition occurs in the channel as shown in Eq. (11) if YU is negative, and channel degradation is calculated with the Eq. (12) if YU is positive:

$$M_{S,dep} = -YU \quad (11)$$

$$M_{S,res} = YU\cdot EK\cdot CVF \quad (12)$$

where $M_{S,dep}$ is the mass of deposited sediments (T), $M_{S,res}$ is the mass of resuspended sediment (MT), EK is the USLE soil erodibility factor, and CVF is the USLE plant cover factor.

Transport of bacteria from streambed sediments to the water column as a consequence of sediment resuspension during high flow events is simulated based on the linear dependence of the total number of released organisms $N_{B,res}$ (CFU) on the mass of resuspended sediment $M_{S,res}$ (MT) (Kim et al., 2010).

$$N_{B,res} = M_{S,res}\cdot C_B \quad (13)$$

where C_B (CFU (MT of sediment)$^{-1}$) is the bacteria concentration in streambed sediments.

The active microbial transport from the streambed sediment to the water column is conceptualized as a groundwater flux-independent phenomenon (Pachepsky et al., 2017; Park et al., 2017). Total number of bacteria released into the overlying water in a day is proportional to the bottom area of the stream reach and the concentration of *E. coli* in the streambed C_B:

$$N_A = \gamma\cdot A_{bottom}\cdot C_B \quad (14)$$

where N_A is the total number of bacteria released from bottom sediment by active transport (CFU day^{-1}), A_{bottom} is the bottom area of the stream reach (m^2), and γ is the bacteria release factor (MT m^{-2} day^{-1}).

The deposition with sediment settling, the net amount of bacteria deposition is calculated using the following equation (Pachepsky et al., 2006; Kim et al., 2010):

$$N_{B,dep} = N_{B,W} \cdot \frac{K_p \cdot M_{S,dep}}{Q_c + K_p \cdot M_{S,W}} \quad (15)$$

$$\log_{10} K_p = -1.6 + 1.98 \cdot \log CLAY \quad (16)$$

where $N_{B,dep}$ is the total number of *E. coli* deposited (CFU), $N_{B,W}$ is the total number of bacteria in water (CFU), K_p is the partitioning coefficient of bacteria between the sediments and water (m^3 MT^{-1}), $M_{S,W}$ is the mass of sediment in water (MT), Q_c is the volume of water in the stream reach (m^3), and *CLAY* is the percentage of clay in sediment (%).

The Q_{10} model is utilized for bacteria die-off and survival in water which is mathematically similar to equation of survival in manures (Blaustein et al., 2013). Water temperature is calculated from average daily water temperature (Stefan and Preud'homme, 1993).

$$\log(N_w) = -k_{s,w} \quad (17)$$

$$k_{s,w}(T_w) = k_{s,w}(20) \cdot Q_{10,w}^{\frac{T_w - 20}{10}} \quad (18)$$

$$T_w = 5.0 + 0.75 \cdot \overline{T}_{av} \quad (19)$$

where $k_{s,w}$ is the rate coefficient which is the function of temperature, T_w is the average daily water temperature (°C), $k_{s,w}(20)$ is the survival rate at 20 °C, the parameter $Q_{10,w}$ reflects the sensitivity of $k_{s,2,w}$ to temperature, and $\overline{T}_{av}$ is the average air temperature on the day (°C).

A stepwise function was used to simulate bacteria concentrations in streambed sediment C_B:

$$\log C_B = \begin{cases} \log C_{B,mean} + H \log \Delta C_B, & j < j_{start} \\ \log C_{B,mean} - H \log \Delta C_B, & j_{start} \le j \le j_{end} \\ \log C_{B,mean} + H \log \Delta C_B, & j > j_{end} \end{cases} \quad (20)$$

where j is the day of year, $\log C_{B,mean}$ is the mean of logarithms of *E. coli* concentrations over the year, respectively, $\log \Delta C_B$ is the half of the annual magnitude of the logarithm of *E. coli* concentration in sediment, respectively, $H = 1$ in southern hemisphere, $H = -1$ in the northern hemisphere, j_{start} is the Julian day when the switch from winter to summer (summer to winter) concentrations occurs in northern (southern) hemisphere, and j_{end} is the Julian day when the switch from winter to summer (summer to winter) concentrations occurs in southern (northern) hemisphere. The use of Eq. (20) is illustrated in Supplementary material 1.

2.4. Coupling the bacteria fate and transport module with the APEX model

The bacteria fate and transport module is coded in FORTRAN for consistency with the parent APEX model and coupled with the APEX model as a subroutine. The bacteria subroutine runs daily, along with other APEX components as part of subarea processes linking bacteria variables dynamically to other internal state variables such as the daily amount of applied or deposited manure, daily temperature, stream reach length, depth, and profile, runoff depth, water yield, amount of manure eroded from a subarea, and amount of the suspended and deposited sediment during the run time. Model parameters listed in Table 1 are read from an input file that is newly added to the APEX model.

Since the bacteria in manure applied on different days have an individual history of survival, erosion is computed separately for each manure application event. For that purpose, the total amount of manure eroded in a day is partitioned to multiple manure pools that are tagged by different deposition days in proportion to daily application amounts. The survival, die-off, and removal of bacteria are computed for each of manure deposition separately. The sum of bacteria amount removed from each deposition pool leads to daily bacteria removal from the field and input to the reach.

3. Evaluating the model with the Toenepi watershed dataset

3.1. Study area

The microbial fate and transport submodule was applied to the Toenepi watershed in the Waikato region of the North Island of New Zealand (Fig. 1). The elevation above mean sea level of study area is between 30 and 130 m. The annual rainfall during 2004–2008 was 1152 mm year^{-1} and the mean air temperature was 14.3 °C. The warmest months are December to February (summer, DJF) and the coldest months are June to August (winter, JJA). From September to November is spring (SON) and from March to May is fall (MAM). The predominant land use is intensive cows grazing all year around. Animal waste is deposited directly onto the land everyday as cows graze pasture. Cow manure from grazing is the main source of bacteria in the surface runoff in this watershed.

3.2. Data acquisition and setup for simulation

Field monitoring was conducted from July 2002 to February 2008. Streamflow and in-stream *E. coli* concentrations at the catchment outlet (site A, Fig. 1) and weather conditions (site B, Fig. 1) were measured and recorded during the monitoring period as described in Wilcock et al. (2006). Farmers in this watershed were surveyed as described in Wilcock et al. (2006) to determine farm management practice parameters for the APEX model. The average stocking rate in 2003 in this study area was 3.1 animal units (AU) ha^{-1} and wet weight manure production was around 40 kg animal^{-1} day^{-1} (Wilcock et al., 2006; Muirhead, 2014; Clague et al., 2015; Muirhead, 2015).

For APEX simulations, spatial data including Digital Elevation Map (DEM), land use, and soil map, weather data, and soil information were obtained from available sources. Based on the auto-delineation in ArcAPEX, the watershed (1538 ha) was divided into 79 subareas and the average subarea size was 20 ha (Fig. 1). The land use spatial data was obtained from (LCDB, 2015) and the grazed pasture would be the dominant land cover (93% of the watershed). The soil shape file and user soil database were acquired from Landcare Research Manaaki Whenua Soil Report (report generated 28-Jul-2015 in http://smap.landcareresearch.co.nz/). Toenepi catchment soils were predominantly volcanic silt loams (Wilcock et al., 1999). The soil database provided the input data for APEX, specifically soil hydrologic group (A, B, C or D), depth to bottom of layer, bulk density, soil water content at wilting point and field capacity, sand, silt and clay content are included.

3.3. Sensitivity analysis

The global sensitivity analysis was performed separately for parameters of the APEX hydrologic module and parameters of bacteria module. This study used the Agricultural Policy Environmental eXtender – auto Calibration and UncerTainty Estimator (APEX-CUTE) 3.0 for sensitivity analysis of hydrology module. The APEX-CUTE was developed for sensitivity analysis and calibration with a user-friendly interface (Wang et al., 2014). We utilized the Morris method (Morris, 1991; Campolongo et al., 2007) for the sensitivity analysis which subdivides each factor range into n intervals of equal probability. Random values of the factors are generated such as each interval is sampled only once for each factor (Wang et al., 2014).

For sensitivity analysis of bacteria module, we applied the method which is a combination of Latin Hypercube and one-at-a time method (LH-OAT). It allows a global sensitivity analysis for a large number of

Table 1
Parameters of the APEX bacterial module.

Symbol	Definitions	Range for sensitivity analysis	Used in simulations	Unit	Global measure of sensitivity	Reference
N_i	Initial number of FIO in animal or manure	$1.7\cdot10^{9}$–$4.9\cdot10^{12}$	$2.2\cdot10^{9}$	CFU (T of manure)$^{-1}$	0.21	Muirhead, 2009
$t_{s,m,1}$	Duration of the first stage of die-off in manure	7–38	7	day	0.00	Park et al., 2016
$k_{s,1,m}$	Survival rate in manure at the first survival stage	−3.8–2.5	0.001	day^{-1}	0.09	Park et al., 2016
$k_{s,2,m}$ (20)	Survival rate in manure at 20 °C at second survival stage	0.005–0.225	0.1	day^{-1}	0.09	Park et al., 2016
$Q_{10,m}$	Temperature sensitivity parameter at the second survival stage in manure	1–2	1.5	—	0.05	Blaustein et al., 2013
k_w	Manure weathering rate coefficient	0–1	0.1	day^{-1}	1.43	Kleinman et al., 2011
k_r	Rate of rainfall-related bacteria growth in manure	0–1	0.58	day^{-1}	0.31	Van Kessel et al., 2007
γ	Low-flow streambed sediment bacteria release factor	$3\cdot10^{-6}$-$7\cdot10^{-5}$	2×10^{-5}	T m^{-2} day^{-1}	1.88	Pachepsky et al., 2017; Park et al., 2017
$k_{s,w}$ (20)	Survival rate at 20 °C in water	0.02–1.0	0.725	day^{-1}	0.35	Blaustein et al., 2013
$Q_{10,w}$	Temperature sensitivity parameter at the survival stage in water	1–2	1.52	—	0.35	Blaustein et al., 2013
$C_{B,mean}$	Average of the logarithms of sediment *E. coli* concentrations in cold and warm periods over the year	1E+6–1E+8	1E + 7	CFU m^{-2}	0.33	Muirhead et al., 2004
$\log\Delta C_B$	Half of the annual magnitude of the logarithm of *E. coli* concentration in sediment	0–1	1	log (CFU m^{-2})	4.63	Kim et al., 2010
j_{start}	Day of the year when sediment concentrations become low	90–150	121	—	2.93	Kim et al., 2010
j_{end}	Day of the year when sediment concentrations become high	244–304	274	—	3.25	Kim et al., 2010

parameters with a limited number of model runs (Van Griensven et al., 2006). The partial effect $S_{i,j}$ is found for the parameter "i" in the j^{th} Latin Hypercube sampling point is. Data from 2004 to 2006 were utilized for the sensitivity analysis.

$$S_{i,j}=\left|\frac{100^{*}\left(\frac{M(e_1,\cdots,e_i\cdot(1+f_i),\cdots,e_p)-M(e_1,\cdots,e_i,\cdots,e_p)}{\frac{[M(e_1,\cdots,e_i\cdot(1+f_i),\cdots,e_p)+M(e_1,\cdots,e_i,\cdots,e_p)]}{2}}\right)}{f_i}\right| \quad (21)$$

where $M(\cdot)$ refers to the model output sensitivity that is studied, f_i is the fraction by which the parameter e_i is changed from the predefined constant. The global measures of sensitivities (S) of each parameter were calculated by averaging these partial effects $S_{i,j}$.

3.4. Calibration and evaluation of the model

The time period from July 2002 to December 2003 was used as the spin-up periods for simulation. Data from 2004 to 2006 were utilized for the model calibration, and data from 2007 to 2008 were utilized for the model validation. Both calibration and validation were conducted separately for hydrology parameters (Table 3) and bacterial parameters (Table 1). The APEX-CUTE 3.0 was utilized for hydrological module calibration using the streamflow monitoring data at the catchment outlet. The model performance was evaluated using the determination coefficient R^2 and the Nash and Sutcliffe (1970) model efficiency (NSE).

The bacteria module was calibrated manually using the monitored *E. coli* concentration in the streamflow at the catchment outlet. Logarithms of concentrations were used in NSE and Root Mean Square Error (RMSE) computations because bacteria data typically follow a log-normal distribution and using logarithms minimizes the influence of outliers present in the data (Desai et al., 2011; Niazi et al., 2015).

The frequency curve analysis method was applied to compare measured and predicted data for bacteria concentrations. This method consists of a statistical comparison of cumulative probability distributions of model errors. It allows evaluation of the quality of the simulation and to compare impacts of different management scenarios (Baffaut and Benson, 2003; Pachepsky et al., 2006; Parajuli et al., 2009; Bougeard et al., 2011).

We assumed that one measured value of *E. coli* concentration on the day "i" represents simulated concentrations averaged over the days from "i − (τ − 1) / 2" to "i + (τ − 1) / 2" where τ is the number of days in the time window encompassing the day of the measurement. This auxiliary parameter was calibrated along with the rate γ of active transport of *E. coli* from the streambed sediment to water column. The Kolmogorov-Smirnov test was used for the distribution comparisons and the *p*-value of the Kolmogorov-Smirnov statistic was a metric of model performance. This phase of calibration was done under assumption of time-independent concentration of *E. coli* in streambed sediment. After γ was found parameters of annual dynamics of *E. coli* in sediment $\log\Delta C_B$, $j_{\max,start}$ and $j_{\max,end}$ (see Eq. 20) were found manually to maximize the percentage of data points in which the deviation of simulated concentration from a measured one was below one order of magnitude.

4. Results

4.1. Hydrological data and simulations

Seasonal precipitation and streamflow are shown in Table 2. Overall, winters had the highest streamflows whereas summers were dominated by baseflow. Falls and springs had large interannual variation of streamflows. In 2008, for example, mostly baseflow was observed in spring, whereas the highest seasonal flows were found in spring of 2005. Unlike spring and fall, the interannual variation of summer and winter flows was not high; the interannual variation coefficient was only 21% for winters and 113% for fall. High precipitation in summers was not translated into high flows. Overall variation in precipitation among seasons was lower than variation in streamflows.

Table 3 shows the hydrologic parameters with their ranges and calibrated values. Runoff curve number (CN) initial abstraction (PARM 20) and CN index coefficient (PARM 42) were the most sensitive parameters that directly affected runoff. Subsurface flow factors (PARM 90) and return flow ratio (RFPO) were sensitive parameters that directly affected baseflow and aquifer recharge. They were followed by groundwater residence day (RFTO), groundwater storage (PARM 40), and maximum groundwater storage (GWSO). Overall, by far the most sensitive parameters for hydrological module were GWSO and PARM 90.

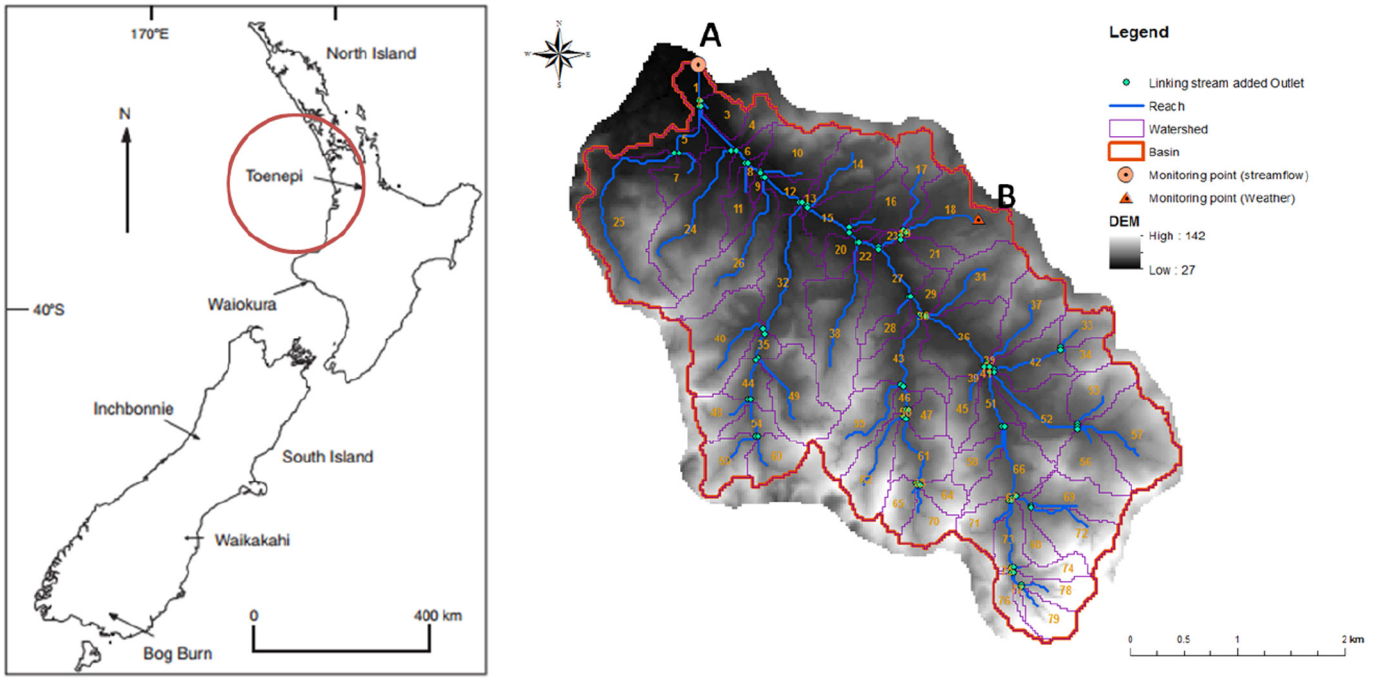

Fig. 1. Map of the Toenepi watershed showing the delineated subareas and the locations of the streamflow and weather monitoring.

Simulated daily streamflow reflected the monitored values well, although streamflow was overestimated under the high precipitation in some cases (Fig. 2). The coefficient of determination (R^2) was 0.63 for the calibration period (2004–2006) and 0.77 for the validation period (2007–2008). The NSE was 0.54 in calibration period (2004–2006) and 0.67 in validation period (2007–2008). According to Moriasi et al. (2007), calibrated hydrological modeling results were satisfactory and acceptable for further analyses.

4.2. E. coli in streamflow data and simulations

Table 4 contains seasonal geometric means of measured *E. coli* concentrations. There was a progressive decrease in annual geometric mean concentrations during the study period. Overall, *E. coli* concentrations during summer baseflow periods are mostly larger than in winters. Geometric mean *E. coli* concentrations in fall and spring have interannual variability higher than those in summer and winter. Seasonal geometric mean concentrations do not exhibit correlations with seasonal average streamflow or precipitation. Interannual variation of spring and fall geometric mean concentrations was higher than that in winter and summer.

Most parameters used in the bacteria simulation were taken from literature and further refined for calibration (Table 1). The exceptions were parameters to find bacteria concentration for streambed sediment C_B in Eq. (20), the rate parameter γ, and the temporal window length τ. Parameters of Eq. (20) were found from the inspection of available in literature data on interannual dynamics of *E. coli* concentrations in sediments and estimated parameters from literature values of seasonal differences in *E. coli* concentrations and reported values for the Toenepi watershed. The detailed explanation is presented in Supplementary materials. The values of parameters were $\log \Delta C_B = 1.0, j_{start} = 121, j_{end} = 274$, and $\log C_{B,mean} = 10^7$ CFU T^{-1}.

The range of the parameter γ was taken between 3×10^{-6} and 7×10^{-5} T m^{-2} day^{-1} based on the Pachepsky et al. (2017) and Park et al. (2017) and the averaging window τ of 1, 3, 5, and 7 days was tried. Results the trials are shown in Table 1. The value of $\gamma = 2 \cdot 10^{-5}$ T m^{-2} day^{-1} provided very good correspondence between distributions of logarithms of simulated and measured values (Table 5). With these parameter values, 89% of the predictions was within one order of magnitude and the rest of the predictions were between 1 and 2 orders of magnitude.

Monitored *E. coli* concentrations and daily simulation results are shown in Fig. 3. Predicted *E. coli* concentrations in streamflow were between 30 and 32,370 CFU 100 mL^{-1}. This range was close to the range of measured values. The distribution of model residuals is shown in Fig. 4. The median residual value of logarithm of concentration ($\log_{10}C$) was 0.01, 0.04, and −0.13 respectively in 2004–2008, calibration period (2004–2006) and validation period (2007–2008). The standard deviation of the residual value of $\log_{10}C$ was 0.63 and 0.84 respectively over the calibration period 2004–2006 and validation period 2007–2008. The model was well calibrated and validated for bacteria simulation with 0.627 and 0.820 of RMSE respectively in calibrated and validated periods. Performance of the model was similar for different seasons. The overall NSE value was 0.33.

Table 2
Average streamflow and precipitation summarized over each season and year.

Year	Precipitation (mm $month^{-1}$)					Streamflow (m^3 s^{-1})				
	Spring	Summer	Fall	Winter	Year	Spring	Summer	Fall	Winter	Year
2004	114	149	62	117	105	0.15	0.06	0.04	0.26	0.13
2005	103	95	85	108	96	0.43	0.06	0.06	0.25	0.20
2006	73	106	147	91	97	0.09	0.02	0.11	0.36	0.14
2007	74	93	73	136	87	0.15	0.02	0.02	0.21	0.10
2008	66	71	102	171	95	0.04	0.01	0.33	0.32	0.19
2004–2008	86	80	94	124	96	0.20	0.03	0.11	0.28	0.15

Table 3
Calibrated APEX model parameters that are most sensitive in hydrological simulations.

Parameters or input	Description	Range	Final chosen value	Process impacted directly	Sensitivity index
GWSO	Maximum ground water storage	5–200 (mm)	15	Recharge/baseflow	0.884
Parm90	Subsurface flow factor	1–100	10	Recharge/baseflow	0.865
Parm 42	CN index coefficient	0.5–2.5	1.383	Runoff	0.438
RFTO	Groundwater residence day	0–365	15.459	Recharge/baseflow	0.322
Parm40	Groundwater storage	0.001–1	0.25	Recharge/baseflow	0.2
Parm20	Runoff CN initial abstraction	0.05–0.4	0.264	Runoff	0.155
RFPO	Return flow ratio (returnflow / (return flow + deep percolation)	0–1	0.5	Recharge/baseflow	0.052
CN2	Initial condition II curve number (CN2)	±5	3	Runoff	0.047

The hypothesis that the simulated and measured concentrations belong to the same statistical distribution was tested with results shown in Fig. 5. The probability of the distribution to be true was 0.46 for the calibration dataset, 0.14 for the validation dataset, and 0.44 for data from all years. Median values of simulated and measured *E. coli* concentrations were around 500 CFU 100 mL^{-1}. Distributions of logarithms of *E. coli* concentrations appeared to be symmetrical.

The results of sensitivity analysis showed the parameters related to the streambed sediment have a higher sensitivity than other parameters. In particular, $\log_{10}\Delta C_B$, j_{end}, j_{start}, and γ have the highest sensitivity for bacteria module (Table 1). Survival rate in water, Q_{10} in water, the manure weathering rate coefficient, and Q_{10} value in manure had relatively lower sensitivity.

Simulated *E. coli* concentrations exhibited seasonality in their dependencies on the streamflow (Fig. 6 and Fig. 7). The summer data demonstrated the well-expressed decrease of the concentrations with the increase in streamflow. However, the trend changed from decreasing to increasing when the streamflow was above 0.01 $m^3\ s^{-1}$ (Fig. 6b and Fig. 7b). The streamflow value of 0.01 $m^3\ s^{-1}$ appeared to be the threshold for spring and fall, too. There was mostly a decrease of concentration with the increase of flow below this streamflow threshold (Fig. 6a and Fig. 7a, Fig. 6c, and Fig. 7c). Both seasons showed the increase of *E. coli* concentration with streamflow above 0.01 $m^3\ s^{-1}$. Winter data indicate the presence of another threshold streamflow value approximately of 1 $m^3\ s^{-1}$. Above this value the decrease in concentrations with increasing streamflow was detected in both calibration and validation datasets (Fig. 6d and Fig. 7d).

The catchment-wide variation of *E. coli* fate and transport variables are shown in Figs. S2 through S4 in Supplementary material. Total catchment *E. coli* reservoir is surprisingly stable around $3.2 \cdot 10^{16}$ CFU (Fig. S2), with only slight decrease occurs in July–August. In Fig. S3, the manure loss during runoff events is on average 0.04 T ha^{-1} which is equivalent to 40 kg or the approximate output from one cow per day. Concentration of *E. coli* in waterways per unit area of the catchment fluctuates substantially by two orders of magnitude. It reflects the coupled effects of both dilution and runoff (Fig. S4).

5. Discussion

The APEX hydrologic module has been calibrated and validated previously. For example, Wang et al. (2009) simulated streamflow and water quality at Shoal Creek, Texas (22.5 km^2) and obtained R^2 values for streamflow from 0.76 to 0.78. Other studies suggest that a range of R^2 between 0.50 and 0.90 was obtained for APEX calibrated flow (Gassman et al., 2010; Wang et al., 2014). In our work, the APEX hydrology module was calibrated with an R^2 of 0.77 for the validation period which compares well with the other published applications.

The bacteria module reproduced the monitored pattern of *E. coli* concentrations at the outlet reasonably well (Fig. 5). Over the calibration periods, 89% of the predictions fell in the range of one order of magnitude from observation and rest of the predictions was between one and two orders of magnitude. Over the validation period, only 70% of the predictions were within 1 order of magnitude and the rest of the predictions were between 1 and 2 orders of magnitude.

It should be noted that model calibrations compare modeled daily average concentrations to instantaneous grab samples collected from the stream. It is likely that some part of this error is due to variation of the grab sample results around the true daily average concentrations, an area of catchment science that is currently scarcely researched.

The performance of APEX in this work was similar or better than in previous studies with the SWAT model. Pandey (2012) and Pandey et al. (2012a) achieved 60% of predictions within one order of magnitude with the bias toward positive deviations. After including temperature-dependent sediment concentrations in SWAT, Pandey et al. (2016) found 83% of predicted concentrations within the one order of magnitude range from measured ones. Benham et al. (2006) developed TMDLs for the Shoal Creek watershed (337 km^2) in Missouri and obtained NSE values of 0.21 to 0.58. Parajuli et al. (2009) simulated source-

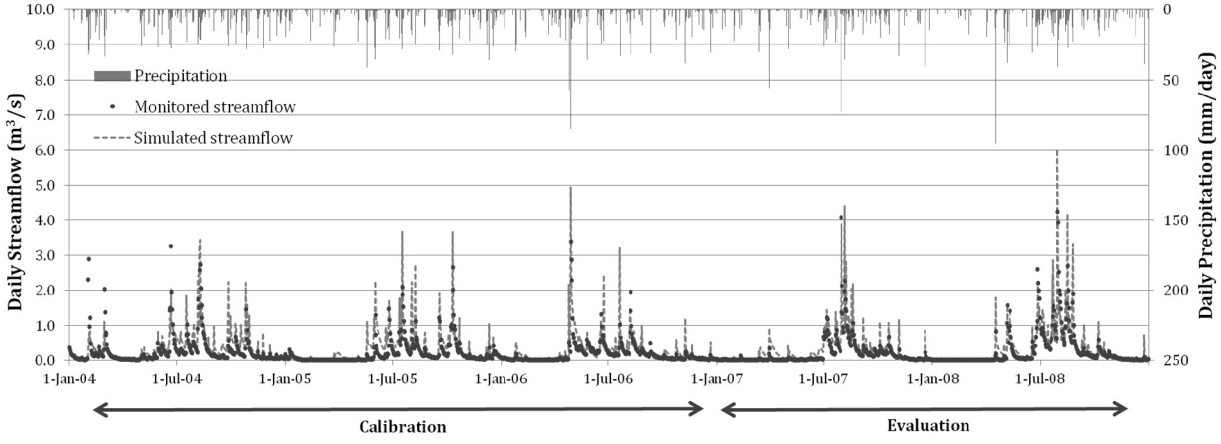

Fig. 2. Measured and simulated daily streamflow at the watershed outlet and precipitation.

Table 4
Geometric mean of measured *E. coli* concentrations summarized for each season and year.

Year	Spring	Summer	Fall	Winter	Year
	(CFU 100 mL^{-1})				
2004	414	364	779	332	444
2005	461	303	1002	206	412
2006	437	448	328	252	357
2007	1761	190	263	53	261
2008	51	335	210	471	256
2004–2008	511	316	449	200	344

Table 5
Results of the search for the streambed sediment bacteria release factor γ.

γ (T m^{-2} d^{-1})	τ = 1 day		τ = 3 days		τ = 5 days		τ = 7 days	
	$P_{K\text{-}S}$[b]	GM[a]	$P_{K\text{-}S}$	GM	$P_{K\text{-}S}$	GM	$P_{K\text{-}S}$	GM
1.0×10^{-5}	0.44	321	0.31	312	0.60	317	0.75	323
2.0×10^{-5}	0.31	391	0.76	381	0.60	389	0.76	398
3.0×10^{-5}	0.09	444	0.44	433	0.32	445	0.21	457

[a] Geometric mean of *E. coli* concentrations over the time window τ days encompassing each day of measurement,
[b] Kolmogorov_Smirnov probability of measured and simulated probability distributions of *E. coli* concentrations being the same.

specific fecal microorganism fate and transport at three watersheds (152 km^2 and smaller) in northwest Kansas and reported NSE values ranging from −2.2 to 0.52. Chin et al. (2009) achieved a NSE of 0.73 at small (15 km^2) Little River watershed in Georgia. A study in France, Bougeard et al. (2011) used SWAT to evaluate the compliance to water quality regulations in the Daoulas Catchment, Brittany, and arrived to the value of NSE is −0.21. Coffey et al. (2013) evaluated applicability of SWAT to predict daily concentrations of *E. coli* in an agricultural catchment Kilshanvey in Ireland (6 km^2) and found values of NSE between −0.42 to 0.29. Overall, APEX in this work performed similarly or better than other models in earlier works.

A possible reason for achieving superior results in this study compared to previous studies might be attributable to the accounting of *E. coli* transfer between streambed sediment and water column during low flow conditions. Previous publications that did not include this mechanism noted the difficulty of matching measured and simulated concentrations in summer time when the base flow dominated. Coffey et al. (2010) noted that during the summer months, corresponding to low flow volumes and less precipitation in this instance, observed concentrations greatly exceed the models predicted concentrations of

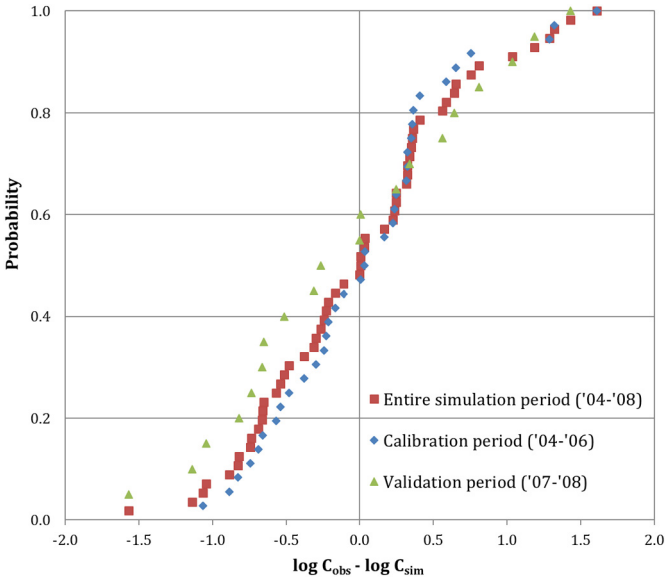

Fig. 4. Cumulative probability distribution functions of the difference between the simulated and measured logarithms *E. coli* concentrations for the whole study period (red squares), model calibration period (blue diamonds) and model evaluation period (green triangles). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

E. coli. Similarly, Kim et al. (2010) reported that the *E. coli* concentrations in the dry season were mostly underestimated at each of their monitoring sites even when the streambed *E. coli* release was accounted for.

The active bacteria transport from streambed to water column, not related to sediment resuspension, that has been so far rarely included in other watershed microbial water quality models (Ghimire and Deng, 2013). Only recently Grant et al. (2012) demonstrated the *E. coli* and enterococci release from the bottom sediments to water without sediment resuspension in turbulent flow along the canal connecting the water treatment plant to a river. Lately the significance of this process for microbial water quality was demonstrated using a library-dependent microbial source tracking approach that matched waterborne *E. coli* isolates to sediment (Piorkowski et al., 2014), modeling with the SWAT model (Park et al., 2017), and direct mass balance measurements (Pachepsky et al., 2017). The importance of this process is in that it can control the microbial water quality during baseflow periods when the major uses of water for irrigation and recreational purposes

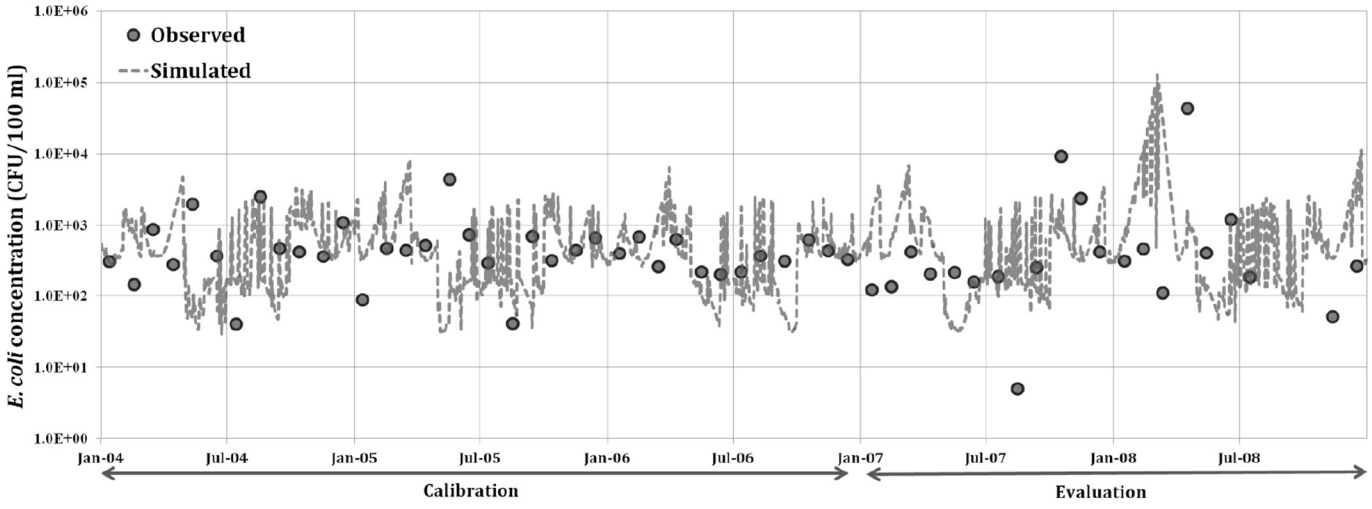

Fig. 3. Observed and simulated *E. coli* concentrations at the outlet of the watershed.

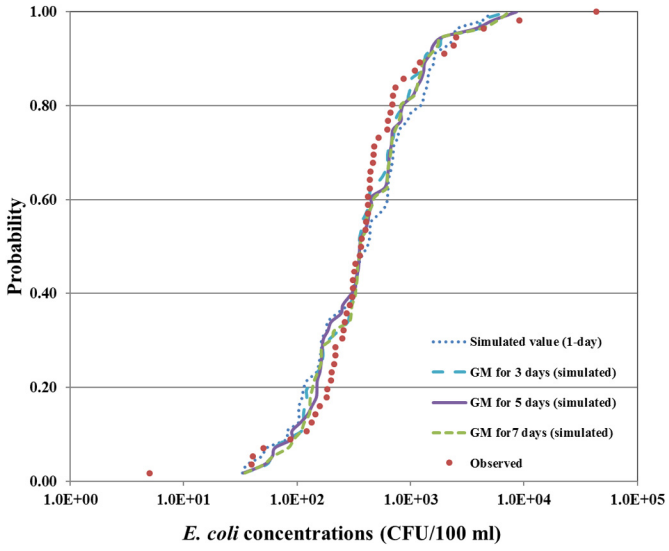

Fig. 5. Cumulative probability distribution of *E. coli* concentrations obtained in simulations, monitoring, and geometric averaging over 3-, 5-, and 7-day time windows encompassing the observation day over entire study period.

take place. The sensitivity analysis in this work showed that the rate constant of the active bacterial transport from streambed to water column γ is one of the most sensitive parameters of the model. So far we know little about the mechanisms and ranges of bacterial fluxes from streambed to water column that occur without sediment resuspension. Grant et al. (2011) provided the hypothetical classification of these mechanisms and invoked the hyporheic exchange as the major reason. Park et al. (2017) distinguished passive transport, i.e., the advective transport of bacteria with groundwater flow through sediment to water column and active transport possible caused by bacterial chemotaxis. Given the importance of water sediment bacterial exchange, one can expect future development of understanding the magnitude, the factors, and the consequence of this phenomenon.

Statistical distributions of simulated and observed concentrations were very similar (Fig. 4). Although the distributions of logarithms of concentration were symmetrical, the hypothesis of log normality was rejected at the 0.001 probability level. The number of very high and very low concentrations was much larger than the lognormal distribution would allow. The distributions had "heavy tails". Whether such distributions are result of analytical or sampling issues, or there are some mechanisms that cause this abnormally high or abnormally low values to appear, presents an interesting avenue for research.

The model of this work does not account for several manure-borne bacteria fate and transport mechanisms, and that potentially can reduce model accuracy. Manure weathering can alter the release and removal rates. Meals and Braun (2006) observed a significant effect of the time between manure application and rainfall on levels of *E. coli* in runoff from agricultural fields. These researchers found that runoff contained ~50% less *E. coli* when manures were applied 3 days prior to rainfall than when applied 1 day prior. They attributed this to bacterial die-off, immobilization of bacteria through adsorption-fixation to surface soils and vegetation, and exposure to ultra violet radiation and desiccation. Vadas et al. (2011) performed a meta-analysis of nine studies involving the release of phosphorous (P) from manures under simulated rainfall and found that in 5 out of 9 studies the increase in time between manure application and rainfall led to reductions in P concentrations in runoff. Fecal bacteria within manure have demonstrated extended persistence in the environment when crusts form on the surface of manure which seems to provide protection from the elements (Muirhead et al., 2005; Soupir et al., 2008). Crusts also can prevent release and removal of

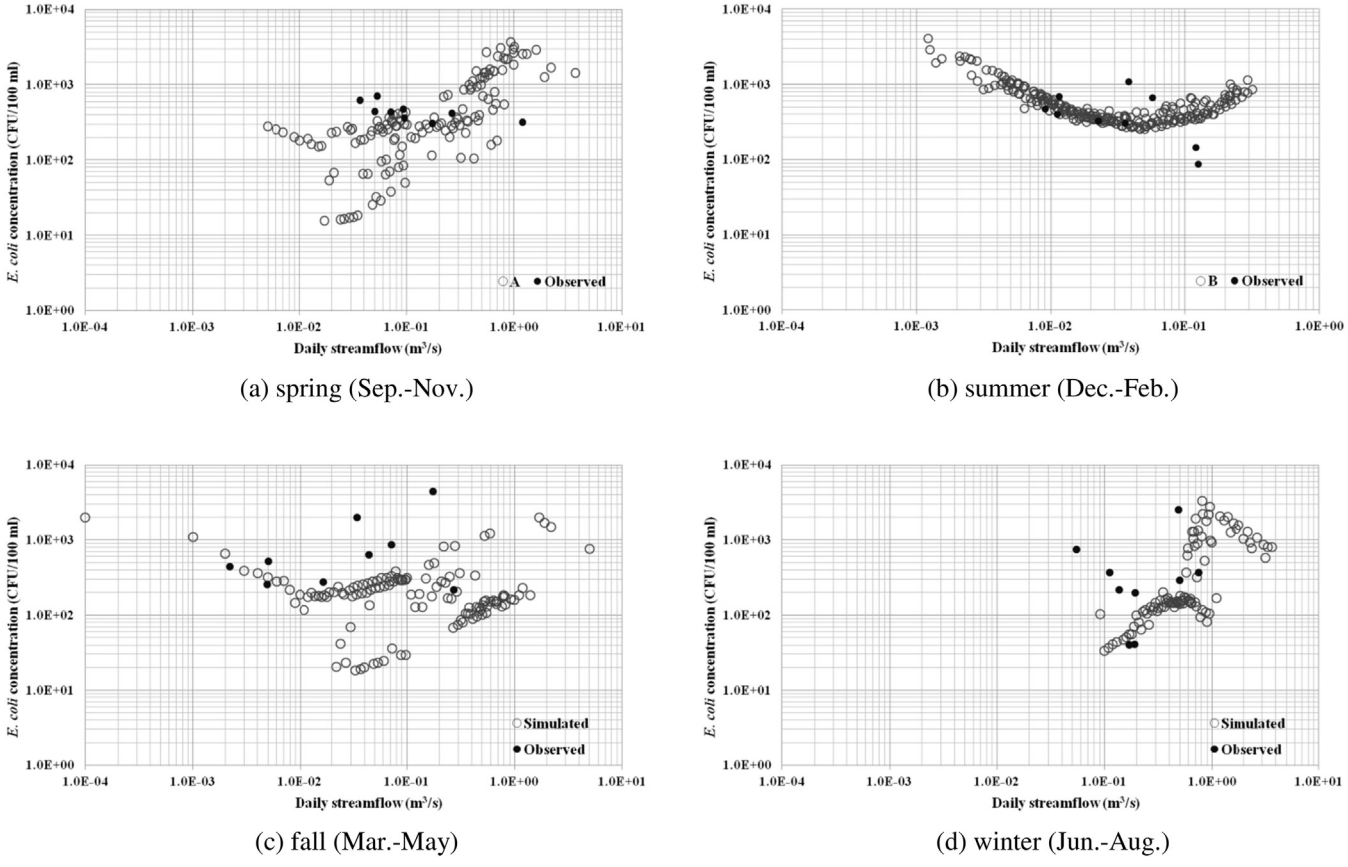

Fig. 6. Seasonality of observed and simulated *E. coli* concentration in their dependencies on the streamflow for the model calibration period.

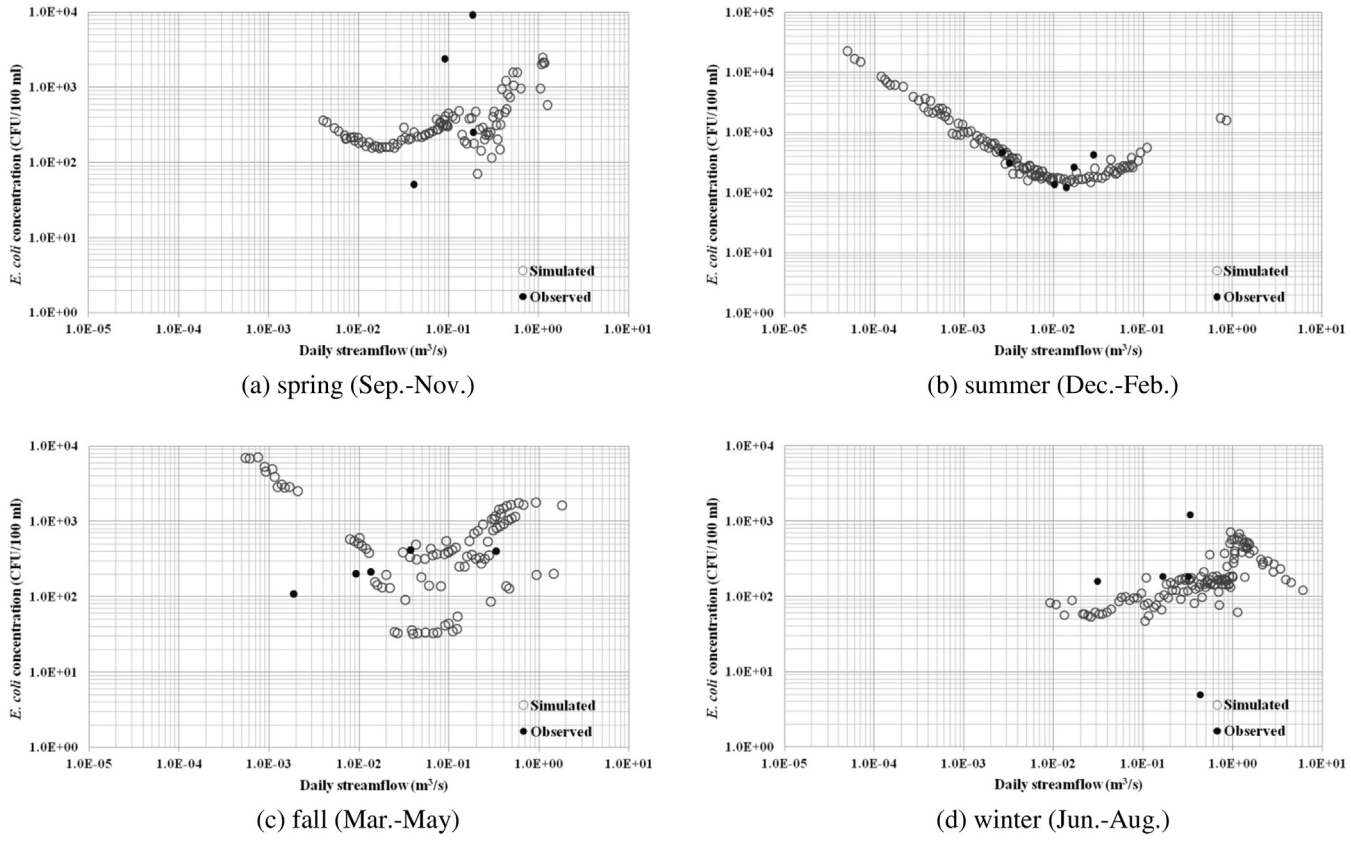

Fig. 7. Seasonality of observed and simulated *E. coli* concentration in their dependencies on the streamflow for the model validation period.

manure constituents including bacteria since a time is needed for crust to soak and become ready to be removed by sheer action of water. The above phenomena were ignored in this work because the k_w parameter has less sensitivity compared with other parameters (Table 1). Some factors of bacteria fate and transport that are known to be spatially or temporally variable are characterized with lumped constant parameters. For example, the clay content in sediment that affects the settling in Eq. (16) is spatially variable, represented by the single value clay content of the dominant soil near the stream reach. A site specific decision has to be made on whether the increase in model accuracy can justify collecting information about such spatial variability.

The accuracy of the model could be affected by animal groups and activities that are currently omitted. The input of *E. coli* from wildlife fecal deposits is currently ignored. Such input was found to be substantial in several studies in U.S. (Cho et al., 2012; Guber et al., 2016). It is difficult to determine accurate numbers of wild animals living or passing through a catchment but earlier farm-scale modeling assumed a density of 4 ducks per km of stream length (Muirhead et al., 2011). Using these numbers, we estimate that the inputs of *E. coli* into the Toenepi stream from ducks would be equivalent to a $1.3 \cdot 10^9$ CFU ha^{-1}which is similar to the flux sediment *E. coli* during baseflow, which ranged from $2.0 \cdot 10^8$–$2.0 \cdot 10^9$ CFU ha^{-1}. The presence of animals wading in streams or coasting near stream banks was also found to be a source of fecal bacteria contributions to stream water (Branham et al., 2005; Parajuli, 2007; Guber et al., 2016). In 1995 there were only 46% of the stream length in the Toenepi that had been fenced off but by 2008 the level of fencing had increased to >80%, with most of this increase occurring between 2001 and 2008 (Wilcock et al., 2013). This change in fencing could be one of the reasons for the improving trend in *E. coli* concentrations observed (Table 4).

The seasonality of *E. coli* concentrations in sediment is simulated in this work with a simple stepwise function. Available data on those concentrations over the year (Kim et al., 2010) shows that although the seasonality is well expressed, the variability is very high and the stepwise linear function (see Eq. (20)) fits the data no worse than the sine function proposed in the (Kim et al., 2010) work. The research of Pandey et al. (2012b) showed that there may be an alternative approach to reproduce the seasonality by applying the temperature-driven growth model and accounting for the sediment *E. coli* population decrease during high flow event. This approach would require data on the response of *E. coli* to nutrients levels in the water column (Shelton et al., 2014). It is possible that model performance can be improved further, if the seasonality in sediment *E. coli* concentrations will be described better. The current knowledge base on this seasonality is poor (Pachepsky and Shelton, 2011; Crabill et al., 1999; Kim et al., 2010) and it's the stepwise description of Eq. (20) that should be eventually refined as more will be learned about the time dependencies of sediment *E. coli* concentrations.

It could be possibly beneficial to consider separate compartments for bacteria in soil and in applied manure, but it is difficult to separate these two compartments in experiments (Muirhead, 2009; Muirhead and Monaghan, 2012). This work follows the tradition of earlier modeling work with animal waste that considered the animal waste “store” on the surface rather than separate soil and manure compartments (e.g., Walker and Stedinger, 1999; Collins and Rutherford, 2004; Wilkinson et al., 2011). Another limitation of the model is the assumption that the overland transport of bacteria is fully coupled with the transport of the eroded manure. It is quite possible that appreciable amounts of bacteria released and transported with runoff during rainfalls can be trapped by soil and vegetation or infiltrated into the soil. Part of the trapped microorganisms can survive and be released and transported with runoff during subsequent rainfalls. Our assumption is that the trapped bacteria are a minor source of bacteria export to surface waters as compared with bacteria in eroded manure. We note that there exists another modeling approach that fully decouples bacteria transport and manure transport (Guber et al., 2011). It includes

simulations of bacteria cell transport with overland flow, as well as sorption by - desorption from top soil layer. This approach requires large number of process parameters. It has been shown to provide a reasonable modeling accuracy when parameters of sorption, desorption, and straining were available from site-specific experiments (Guber et al., 2014). Testing its applicability at the watershed scale can be an interesting future development.

The APEX manure erosion model that drives bacteria fate and transport in this work, is quite elaborate and flexible. Models that work at larger scales, such as SWAT or HSPF, relate bacteria release and bacteria concentrations with a linear function. Linking the *E. coli* losses to the existing manure erosion module in APEX may present advantages for future modeling of manure management mitigation options by allowing for associated co-benefits of nutrient reductions from the same mitigation. This is consistent with the spatial scale of APEX as being a small (farm) scale model that is developed to perform detailed simulation of farm operation and environment. Unlike the large-scale watershed models with fewer details on simulating agricultural managements, APEX allows for simulating detailed management practices under various strategies. According to Srivastava et al. (2007), APEX is one of the few existing models that are capable of simulating flow and pollutant transport routing at the field scale. The range of scales at which APEX can operate, starts from individual fields and ends at watersheds subdivided into with subareas connected by routing water, chemicals, and now bacteria among subareas and channel systems. Other areas for future development include the incorporation of "non-hydrology driven inputs" such as the direct deposition of *E. coli* to the stream from farm or wild animals or other point sources.

6. Conclusion

In this study, a bacteria module was developed and integrated into the APEX model for simulating the fate and transport of manure-borne bacteria on the landscape and in streamflow. The model is demonstrated to be useful for investigating site-specific microbial contamination, developing management practices, and making decision and regulations for bacteria control. The submodel developed considered release from manure, survival and die-off of bacteria, transport in runoff and in-stream processes. The submodel was coded in FORTRAN which is compatible with APEX model and applied to the Toenepi watershed in the Waikato region of the North Island of New Zealand. Most of parameters for this simulation were taken from literature rather than calibrated. Only the parameters for streambed sediment were calibrated which showed high sensitivity for microbial submodel. Distributions of simulated and observed concentrations were very similar. Overall, APEX in this work performed similarly or better than other models in earlier works.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2017.09.231.

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