Water Air Soil Pollut (2016) 227:351
DOI 10.1007/s11270-016-3053-2

Impact of the Linked Surface Water-Soil Water-Groundwater System on Transport of *E. coli* in the Subsurface

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Received: 8 March 2016 / Accepted: 17 August 2016

Abstract *Escherichia coli* (*E. coli*) contamination of groundwater (GW) and surface water (SW) occurs significantly through the subsurface from onsite wastewater treatment systems (OWTSs). However, *E. coli* transport in the subsurface remains inadequately characterized at the field scale, especially within the vadose zone. Therefore, the aim of this research is to investigate the impact of groundwater fluctuations (e.g., recharging, discharging conditions) and variable conditions in the vadose zone (e.g., pulses of *E. coli* flux) by characterizing *E. coli* fate and transport in a linked surface water-soil water-groundwater system (SW-SoW-GW). In particular, this study characterizes the impact of flow regimes on *E. coli* transport in the subsurface and evaluates the sensitivity of parameters that control the transport of *E. coli* in the SW-SoW-GW system. This study was conducted in Lake Granbury, which is an important water supply in north-central Texas providing water for over 250,000 people. Results showed that there was less removal of *E. coli* during groundwater recharge events as compared to GW discharge events. Also, groundwater and surface water systems largely control *E. coli* transport in the subsurface; however, temporal variability of *E. coli* can be explained by linking the SW-SoW-GW system. Moreover, sensitivity analysis revealed that saturated water content of the soil, total retention rate coefficient, and hydraulic conductivity are important parameters for *E. coli* transport in the subsurface.

Keywords *E. coli* transport · Seasonal variability · Septic tanks · Surface water and groundwater interaction

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1 Introduction

Water resources are prone to microbial contamination in rural areas, where a large number of onsite wastewater treatment systems (OWTSs) are present. Onsite/decentralized wastewater treatment systems serve approximately 25 % of US households and almost 40 % new developments (USEPA 2005; Dwivedi et al. 2008; Lowe and Siegrist 2008). The most common OWTS involves a septic tank unit followed by dispersal to a subsurface soil infiltration unit. Onsite systems are one of the many known contributors of pathogens and nutrients to groundwater (GW) (USEPA 2002). *Escherichia coli* (*E. coli*) is a microbe of fecal origin. Therefore, water contamination by various strains of *E. coli* is becoming common in rural areas in the USA (Bradford et al. 2006; Dwivedi et al. 2013).

The level of *E. coli* contamination to GW depends on multiple factors such as precipitation pattern, thickness

Published online: 31 August 2016

and composition of the vadose zone (Williams et al. 1998), and subsurface heterogeneity (Spalding and Exner 1993; Dwivedi and Mohanty 2016). Physical processes that control the fate and transport of *E. coli* have been studied extensively (Haznedaroglu et al. 2008). Smith et al. (1985) demonstrated that the extent of *E. coli* transport largely depends on soil structure. The authors further suggested that flow through soil macropores, which bypasses the retentive capacities of the soil matrix, is a common phenomenon. Gagliardi and Karns (2000) discussed the impact of soil type and method of pathogen delivery on *E. coli* transport in the subsurface. Another study conducted in a karstic aquifer described that the residence time of *E. coli* in the subsurface, which is correlated with the pore velocity, is crucial for GW contamination (Personne et al. 1998). Furthermore, there is evidence in the literature that the survival and transport of *E. coli* in the subsurface is controlled by various factors, such temperature, rainfall, soil type, porosity, and soil water (SoW) content (Federle et al. 1986). Moreover, hydrological interactions between surface water (SW) bodies, SoW, and GW are of fundamental concern to the migration of contaminants (*E. coli*) in a linked surface water-soil water-groundwater (SW-SoW-GW) system (e.g., McMahon et al. 1995; Bethune et al. 1996). However, despite the importance of SW-SoW-GW interaction, the characterization of the impact of GW flow patterns, due to dynamic boundary conditions, on fate and transport of *E. coli* near surface water bodies is still lacking. Therefore, the goal of this study is to investigate how the interaction of surface water, soil water, and GW affect *E. coli* transport in the subsurface.

To clearly distinguish the impact of these interactions, we model *E. coli* transport in the subsurface—first with representing groundwater and surface water system only and then with linked SW-SoW-GW system, in other words by explicitly representing vadose zone processes in the model. To investigate and capture the impact of surface water-groundwater interactions, we chose MODFLOW because of its capability to simulate lake-groundwater interactions or fluctuating lake levels (Anderson 1991). However, the influence of the vadose zone is oversimplified in MODFLOW, as recharge and concentration boundary conditions are calculated outside the model without appropriate consideration of the vadose zone (Twarakavi et al. 2008). On that account, to understand the transport of *E. coli* in the subsurface under dynamic boundary conditions for a linked SW-SoW-GW system, we use HYDRUS and MODFLOW/MT3DMS models, in which HYDRUS is used to produce *E. coli* flux at the water table that becomes a boundary condition for GW flow and transport. The aim of this research is to investigate *E. coli* transport in the vadose zone under recharging-discharging GW that involves variations in GW table. Besides, this study tests the robustness of model parameters (by using calibrated MODFLOW/MT3DMS parameters without further modification) and characterizes parameter sensitivity to identify dominant controls on the fate and transport of *E. coli* in the saturated zone and SW-SoW-GW system.

2 Study Site

2.1 Site Description

This study is conducted at a water-quality monitoring station (Segment ID: 1205; latitude 32° 27′ 40″ and longitude 97° 42′ 53″) in the Lake Granbury area, which is monitored by the Brazos River Authority. Lake Granbury is a man-made lake of 35 km^2 within the Middle Brazos-Palo Pinto watershed (USGS Cataloging Unit: 12060201). The watershed is a part of the Brazos River basin and is located in north-central Texas, in Hood County. Summers are long and hot while winters are short and mild. Average temperatures range from a low of 1.1 °C in January to a high of 35.5 °C in July. The average precipitation in the watershed is 0.76 m yearly. The watershed has a diversified land use from urban to agriculture; about 31 to 40 % of the land is considered prime farmland. The landscape is described by rolling hills of pasture and cropland surrounded by deciduous forest. Lake Granbury is an important source of water supply in this area, providing water for over 250,000 people in more than 15 cities. Recent studies by the Brazos River Authority (BRA), Texas Water Resources Institute (TWRI), and Espey Consultants, Inc. have concluded that some of the Lake Granbury's coves especially shallow bodies of water are contaminated with *E. coli*.

Several studies have been conducted to assess potential *E. coli* sources in lake or canals in the Lake Granbury Watershed (Riebschleager et al. 2012; Dwivedi et al. 2013). Potential *E. coli* loads can stem from several sources, including livestock (e.g., cattle, pets), malfunctioning septic systems or onsite wastewater treatment systems (OWTSs), surface runoff, and wastewater treatment plants (WWTPs). The nearby WWTP is located in downstream of the study site and thus is not a source. In addition, pets are primarily kept in homes, and pet waste is disposed directly to solid waste management (to landfill mostly via garbage collection). The other livestock is infrequently sighted. Previous studies in the watershed have demonstrated that point source loadings (e.g., OWTSs) are constant, whereas nonpoint source loadings are associated with high flows due to runoff events (Riebschleager et al. 2012). As runoff begins, *E. coli* concentration increases in the lake and canal, which decreases at a faster rate than the river discharge, eventually approaching background levels (Pachepsky and Shelton 2011). Therefore, we applied *E. coli* loads from the malfunctioning septic systems as the primary source of *E. coli* in this system. Moreover, in the Lake Granbury area, these septic systems are located in a zone, where shallow groundwater and surface water interact. Thus, shallow groundwater in the region can be easily contaminated by the sewage and can further contaminate the lake and canal.

2.2 Data Description

The site was characterized for soil texture and shallow subsurface hydrologic conditions (e.g., groundwater level). Seventeen soil cores were carefully excavated from 0.15 to 1.0 m depth at several locations along the *A*-*A*′ transect (Fig. 1). Saturated hydraulic conductivity, bulk density, and soil texture details were obtained by laboratory experiments conducted on these undisturbed soil cores. In particular, saturated hydraulic conductivity for each core was measured based on the constant-head permeameter method (Klute and Dirksen 1986; Mallants et al. 1997). In this method, a hydraulic head on top of the cores is imposed, and the resulting flux is measured at the free-water outlet. Subsequently, soil texture analysis was performed using the hydrometer method (Milford 1997; Lesikar et al. 2005). For soil type, particle-size data were used to classify the soil texture from the USDA textural triangle (Davis and Bennett 1927; Twarakavi et al. 2010). The soil texture varied from silt clay loam to sandy clay loam.

Precipitation data were acquired from the National Climatic Data Center (NCDC) (http://www.ncdc.noaa.gov/), and evapotranspiration data from TexasET Network (http://texaset.tamu.edu/index.php). The Brazos River Authority and the Texas Commission on Environmental Quality (TCEQ) collected the water quality data in Lake Granbury under Clean River Programs (CRP) on Environmental Quality. Concentration data of *E. coli* (CFU/100 mL) in Lake Granbury were available from July 2002 to August 2010 , using grab samples collected monthly at 0.3 m below the surface. The *E. coli* concentration data was measured using the Colilert (Defined Substrate Technology) method (Eaton et al. 1988). The *E. coli* observations used in this study meet all quality assurance requirements (e.g., holding time) of the CRP and the Brazos River Authority Environmental Services. However, we acknowledge the uncertainty in the observed *E. coli* data due to lack of replicates.

3 Methodology

For this study, we modeled *E. coli* transport in the subsurface using MODFLOW/MT3DMS to simulate groundwater and surface water interactions and then with loosely coupled HYDRUS and MODFLOW in a 2-D system to simulate SW-SoW-GW interactions. In the subsequent sections, we provide a description of the conceptual model for the fate and transport of *E. coli* in the subsurface and modeling framework in the Lake Granbury area using the saturated zone (MODFLOW/MT3DMS) and unsaturated zone (HYDRUS-2D) models. We also describe the sensitivity analysis that was performed to identify parameters that control the transport of *E. coli* in the SW-SoW-GW system. For a comprehensive analysis of temporal variability in *E. coli*, we analyzed two different hydrologic scenarios that are possible in the Lake Granbury area:

1. The first scenario (scenario 1) involves the GW level to be lower than the water level in the lake and the canal.
2. The second scenario (scenario 2) involves the GW level to be higher than the water level in the lake and the canal.

The GW table fluctuates in response to climatic conditions (precipitation and water loss due to

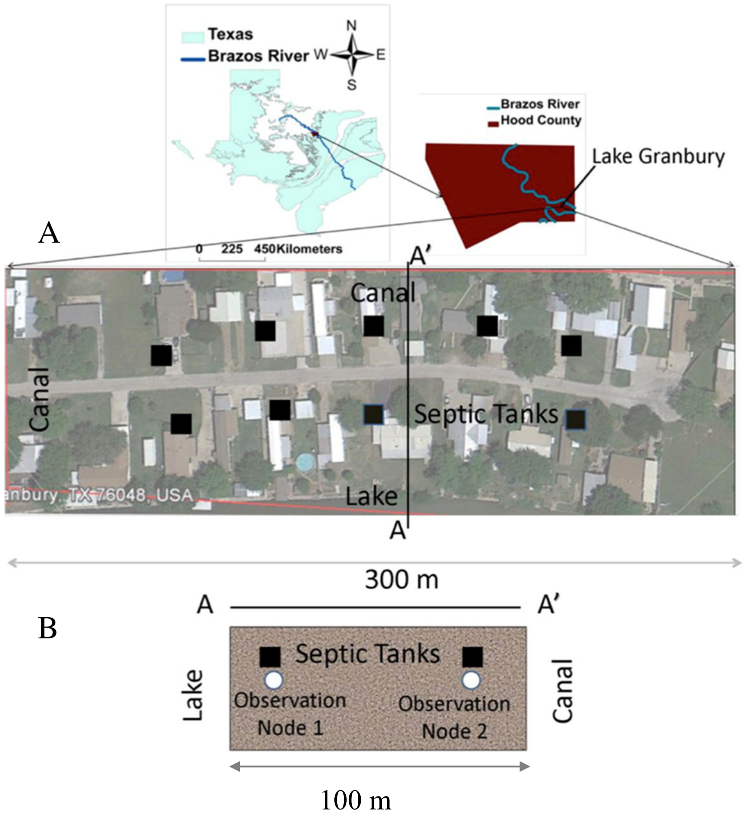

Fig. 1 Plan view of the model domain (m) for **a** MODFLOW/MT3DMS and **b** cross-sectional view of the model domain (m) for HYDRUS-2D along the *A-A′* transect (map courtesy: Google Earth)

transpiration through capillarity), and this fluctuation imposes a dynamic boundary condition in the linked surface water-soil water-groundwater system (Lake Granbury Area). These scenarios allowed us to investigate the possible effects of different hydrologic conditions and resulting temporal variability in the transport of *E. coli* in the subsurface.

3.1 *E. coli* Transport in Porous Media

The advection-dispersion-sorption (ADS) equation is used to describe the fate and transport of *E. coli* in porous media (Matthess et al. 1988; Murphy and Ginn 2000; Powelson and Mills 2001; Pang et al. 2004; Foppen et al. 2005; Foppen and Schijven 2006). The deposition profile of *E. coli* in porous media is modeled as colloid particles (Bradford et al. 2006; Foppen and Schijven 2006). The dynamics of colloid deposition and blocking can be described by expressing colloid transport equation in terms of particle concentration instead of mass concentration (Wan and Wilson 1994; Johnson and Elimelech 1995; Sun et al. 2001) along with terms for straining, attachment, detachment, and die-off (Cunningham et al. 1991; Bergendahl and Grasso 2000; Bhattacharjee et al. 2002; Tufenkji et al. 2004; Torkzaban et al. 2006; Tufenkji 2007)

$$\frac{\partial C}{\partial t} = \nabla.(\mathrm{D}\nabla C) - \nabla.(\mathrm{v}C) - \frac{f}{\pi a_\mathrm{p}^2}\frac{\partial S}{\partial t} - k_\mathrm{i}C \qquad (1)$$

where C is the number concentration (or concentration interchangeably in this study) of suspended bacteria in the aqueous phase $[\mathrm{L}^{-3}]$, $\mathbf{D}$ is the hydrodynamic dispersion coefficient $[\mathrm{L}^2\mathrm{T}^{-1}]$, $\mathbf{v}$ is the pore water flow velocity $[\mathrm{LT}^{-1}]$, f is the specific surface area of the porous medium $[\mathrm{L}^{-1}]$, a_p is the diameter of the bacteria [L], S is a dimensionless quantity that describes the fractional surface coverage and is defined as the ratio of the total cross-sectional area of deposited bacteria and interstitial surface area of the porous medium (Sun et al.

2001), k_i is the die-off rate coefficient of bacteria in the water [T^{-1}], and t is time [T].

For bacteria retained by the solid matrix, several authors (Matthess et al. 1988; Harvey and Garabedian 1991; Lindqvist and Bengtsson 1991; Lindqvist et al. 1994; Powelson and Mills 2001; Pang et al. 2004) assume some percentage available for instantaneous sorption (S_1) and some percentage of bacteria available for kinetic or rate-limited sorption (S_2). On the contrary, some (Tan et al. 1994; McCaulou et al. 1995; Hendry et al. 1999) assume only kinetic sorption (S_2). The instantaneous sorption can be modeled using the partition coefficient (K_d) [MM^{-1}]; the kinetic sorption can be modeled using the first-order kinetics parameterized by the attachment (k_a) [T^{-1}] and detachment (k_r) [T^{-1}] coefficients. Some studies have demonstrated that the kinetic sorption is limited by the blocking (i.e., the occlusion of collector surface) (Ryan and Elimelech 1996), and the effect of the blocking behavior, a dimensionless function (B) of kinetically sorbed *E. coli* (i.e., $B(S_2)$) can be accounted for by employing the Langmuirian dynamics (Johnson and Elimelech 1995; Foppen and Schijven 2006). However, apart from the instantaneous and kinetic sorption models, others (Bradford et al. 2003; Foppen et al. 2005; Bradford and Bettahar 2005; Foppen and Schijven 2006) assume a kinetic fraction also available for straining (S_3), which is modeled using the first-order kinetics parameterized using the straining rate coefficient (k_{str}) [T^{-1}]. Taking all these processes into account, the mass balance equation for retained bacteria can be expressed as

$$\frac{\partial S}{\partial t} = \frac{\partial S_1}{\partial t} + \frac{\partial S_2}{\partial t} + \frac{\partial S_3}{\partial t} - k_{is}S \tag{2}$$

$$\frac{\partial S}{\partial t} = \pi a_p^2\left\{K_d\frac{\partial C}{\partial t} + (k_a B(S_2) + k_{str})C\right\} - k_r S_2 - k_{is}S \tag{3}$$

where k_{is} [T^{-1}] is the inactivation or die-off rate coefficient of bacteria on the solid matrix.

Several studies have noted that equilibrium adsorption and blocking have little impact on *E. coli* transport in the subsurface (Butler et al. 1954; Bouwer et al. 1974). Additionally, various field studies reported that detachment is insignificant at the field scale (Sinton et al. 1997, 2000; Foppen and Schijven 2006). Given the little apparent impact of detachment, inactivation of sorbed cells becomes irrelevant, and Eq. (2) can be reduced to:

$$\frac{\partial S}{\partial t} = \pi a_p^2(k_a + k_{str})C \tag{4}$$

$$\frac{\partial C}{\partial t} = \nabla.(\mathrm{D}\nabla C) - \nabla.(\mathrm{v}C) - f(k_a + k_{str} + k_i)C \tag{5}$$

$$\frac{\partial C}{\partial t} = \nabla.(\mathrm{D}\nabla C) - \nabla.(\mathrm{v}C) - k_{total}C \tag{6}$$

where k_{total} [T^{-1}] is the total retention rate coefficient, which includes the effect of favorable and unfavorable attachment, as well as straining and die-off or inactivation. Although it is desirable to include the effects of abiotic and biotic factors on the total retention of *E. coli*, we used the total retention rate coefficient without distinguishing the impact of these factors, as the distinction between the underlying processes is not possible with the limited data. For this reason, we perform sensitivity analysis and test the reliability of the available model parameters (see Section 3.4).

3.2 Physical Domain Setup for the Saturated Zone

The MODFLOW/MT3DMS model domain is described in Fig. 1a. The flow and transport processes were simulated using 1 m × 1 m uniform grids. The model included one layer, for a total modeling depth of 10 m. Model topography was imported from surveyed elevation data. The top of the model is assigned as a recharge boundary. The initial time step was chosen as 8.64×10^3 s, while the minimum and maximum time steps of 8.64×10^2 and 4.32×10^4 s were employed, respectively. The lateral limits are defined by physical and hydraulic boundaries (Fig. 1).

The flow and transport parameters used for MODFLOW/MT3DMS models are listed in Table 1. The total retention rate coefficient varies in a wide range. For sandy grain size and *E. coli* (1–3 μm), the total retention coefficient is in the order of 6×10^{-4}/h (or 2.16/s) (Foppen and Schijven 2006). Similarly, Pang et al. (2004, 2006) also showed that the removal rate

Table 1 Initial input parameters for *E. coli* transport in SW-SoW-GW

	Value	Reference
HYDRUS parameters		
Lateral dispersivity (m)	1	Gelhar et al. (1992)
Vertical dispersivity (m)	0.1	Gelhar et al. (1992)
Lateral hydraulic conductivity (m/s)	3.5×10^{-8}	Laboratory-measured value
Vertical hydraulic conductivity (m/s)	3.5×10^{-9}	Laboratory-measured value
Total retention coefficient (1/s)	1×10^{-4}	Foppen et al. (2005), Pang et al. (2006)
E. coli concentration in septic tanks (CFU/100 mL)	1×10^{6}	Riebschleager et al. (2012)
Effluent loading (m^3/s)	1.05×10^{-5}	Based on Texas Administrative Code
MODFLOW/MT3DMS parameters		
Total retention coefficient (1/s)	1×10^{-4}	Foppen et al. (2005), Pang et al. (2006)
Effective porosity	0.3	Mace et al. (2000)
Diffusion coefficient (m^2/s)	2.7×10^{-8}	Foppen et al. (2007)

of *E. coli* for silt loam, sandy loam, and sand is of the order of 6×10^{-4}/h (or 2.16/s). In this study, we assumed the total retention rate coefficient, which also includes the effect of favorable and unfavorable attachment, as well as straining and die-off or inactivation, as 6×10^{-4}/h (or 2.16/s).

Visual MODFLOW and MT3DMS models were run under quasi-steady state and then calibrated to observed *E. coli* concentrations using the parameter estimation (PEST) software. This calibration for estimating *E. coli* concentration was done for a period of 49 months—July 2002 to July 2006 at the observation point located by the lake. Model calibration consisted of modifying the flow and transport parameters to minimize the normalized root mean squared (NRMSE) error between estimated and observed *E. coli* concentrations. The model was then run for a period of 49 months—August 2006 to August 2010, without further calibration. These calibrated model parameters were applied to the linked SW-SoW-GW system without further modification.

3.3 Modeling Framework in the Unsaturated Zone and Linked SW-SoW-GW System

E. coli transport in the subsurface was explored in the Lake Granbury area using the physically based HYDRUS-2D hydrologic simulation solver (Šimůnek et al. 2006). HYDRUS-2D allows the user to analyze fate and transport of *E. coli* through saturated, variably saturated regions with complex geometries, and composed of nonuniform soils. In the Lake Granbury area, there are shallow canals, which are hydrologically connected to the lake (Fig. 1).

The modeling domain is described in Fig. 1b. Two-dimensional model domain is 100 m (*X*) by 2 m (*Z*). The model domain is uniformly discretized with 1 m horizontal (*X*) resolution and 0.25 m vertical (*Z*) resolution using unstructured finite element mesh in HYDRUS. An initial time step of 8.64×10^3 s day and minimum and maximum time steps of 8.64×10^2 and 4.32×10^4 s were employed (similar to MODFLOW/MT3DMS). The flow and transport simulations for *E. coli* were performed for a period of 700 days. This simulation period was chosen based on the time required for *E. coli* to reach the peak concentration at observation nodes (Fig. 1). Flow and transport parameters used in the HYDRUS-2D model are listed in Table 1. The boundary conditions are listed in Table 2.

Baseline simulations (scenarios 1 and 2) with no background *E. coli* concentration, as initial conditions, and forcing data (Fig. 2) were run for 2 years in HYDRUS. The simulation reached a steady state in this time frame for two scenarios individually. *E. coli* flux at the water table was calculated using HYDRUS. For the linked SW-SoW-GW system, *E. coli* flux served as the solute (contaminant) boundary condition for GW flow and transport (MODFLOW/MT3DMS). The calibrated model

Table 2 Boundary conditions (BC) for the HYDRUS and MODFLOW/MT3DMS models

	Boundary conditions
HYDRUS	
Hydrologic upper BC	Atmospheric BC
	$q(t) = \begin{matrix} 0 & \text{for } h(t,z) < 0 \\ q(t,x,z) & \text{for } h(t,z) \geq 0 \end{matrix}$
Hydrologic lower BC	Deep drainage
	$q(t) = \begin{matrix} 0 & \text{for } h(t,z) < 0 \\ q(t,x,z) & \text{for } h(t,z) \geq 0 \end{matrix}$
Hydrologic lateral BCs	Variable head
	$h = h(t)$
Solute upper BC	No flux
	$q_c = 0$
Septic tanks BC	Constant flux
	$q_c = q_{c0}$
Solute lateral and lower BCs	Flux type
	$q = q_c(t)$
MODFLOW/MT3DMS	
Hydrologic upper BC	Atmospheric BC
	$q(t) = \begin{matrix} 0 & \text{for } h(t,z) < 0 \\ q(t,x,z) & \text{for } h(t,z) \geq 0 \end{matrix}$
Hydrologic lower BC	Deep drainage
	$q(t) = \begin{matrix} 0 & \text{for } h(t,z) < 0 \\ q(t,x,z) & \text{for } h(t,z) \geq 0 \end{matrix}$
Lateral BCs	Head-dependent flux boundary
	$q(t) = -K(h - h_{\text{ref}})$
Solute upper BC	Flux type
	$q_c = q_c(t)$
Solute lower BC	Flux type
	$q_c = q_c(t)$
Solute lateral BCs	Flux type
	$q_c = q_c(t)$

parameters from MODFLOW/MT3DMS were used in this loosely coupled simulation so as to test the robustness of these model parameters. As suggested above, we considered multiple scenarios that can alter the *E. coli* concentration at the boundary (interface of the saturated and unsaturated zones). Modeling results (*E. coli* estimation) were tested against observations at the monitoring stations.

3.4 Calibration and Sensitivity Analysis

The aim of the sensitivity analysis was to identify model parameters that impact *E. coli* flow and transport in the subsurface as well as to find critical values of parameters that may lead to a reasonable agreement between estimated and observed *E. coli* values. We used a parameter estimation package called PEST, which is model independent. *E. coli* concentrations were available at the water quality monitoring station in Lake Granbury, and therefore, PEST was used for both calibrating the MODFLOW/MT3DMS and performing the sensitivity analysis.

We also analyzed sensitive parameters for HYDRUS-2D, which was used for 2-D flow and solute transport representations in the unsaturated zone. The sensitivity analysis was carried out by individually varying one-factor-at-a-time (OFAT). The OFAT approach has been deemed appropriate for evaluating the sensitivity of different parameters, and this method is computationally frugal that changes one parameter at a time from reference parameter sets, and computes the

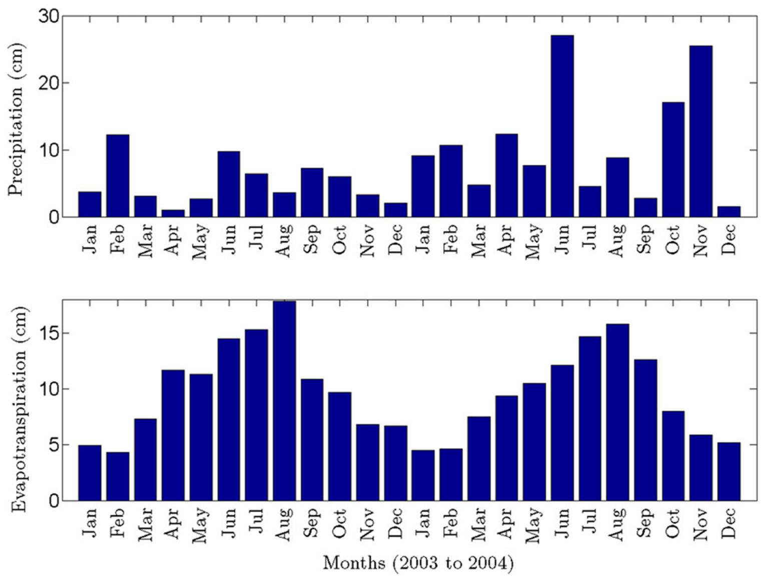

Fig. 2 Precipitation and evapotranspiration in the Lake Granbury area for 2003 and 2004 demonstrate that June to September have high evapotranspiration and lower precipitation as compared to October to May (data: Texas Water Development Board)

difference in the outputs (Arora et al. 2012). The OFAT approach involved perturbing each factor individually within a reasonable interval (±30 %) and keeping the rest of the factors constant at their baseline values.

4 Results and Discussion

4.1 *E. coli* Transport in the Subsurface

The base case simulation was designed to consider groundwater and surface water system (MODFLOW/MT3DMS) only so as to gain insight into the interpretation of processes controlling *E. coli* transport in the saturated zone. Simulation results (not shown here) were able to capture the average *E. coli* concentrations but failed to capture the variability in time. Simulation results showed that groundwater and surface water systems largely control *E. coli* transport in the subsurface. The normalized mean squared error (NMSE) value was >0.95 from the simulated and observed *E. coli* concentrations. It is worth mentioning that the lower the NMSE, the better the model performance. An NMSE of 0 indicates that the model predictions are perfect.

To gain insights into the temporal variability of *E. coli* concentrations, we used autocorrelation function (ACF) and partial autocorrelation function (PACF) to describe the seasonal occurrence of *E. coli* in the lake. The ACF describes the similarity between *E. coli* observations as a function of the time lag between them. The higher ACF values show repetitive patterns, such as seasonality. The PACF computes the partial correlation with its lagged values in a time series. Figure 3 demonstrates ACF and PACF of measured *E. coli* in the lake. Repeating patterns of 7 and 10 months are observed. This is because climatic seasonality has an effect on *E. coli* transport. Seasonality also has an impact on GW table that fluctuates in response to climatic conditions. For example, in Lake Granbury site, winter (October to May) precipitation is often higher than summer (June to September) precipitation (Harmel et al. 2003), and so GW storage is not fully recharged in summer. This is also apparent in Fig. 2 where higher precipitation and lower evapotranspiration are observed in winter months for the years 2003 and 2004. We will evaluate the role of seasonal groundwater fluctuations on *E. coli* fate and transport (Section 4.2).

Because the presence of *E. coli* in the lake is a continuous phenomenon, it is appropriate to test our model performance against smoothed out *E. coli* data. Based on the ACF and PACF analysis, a 3-month moving average (frequency is 3 months after winter months) of *E. coli* concentrations was selected. The NMSE value was 0.77 from the observed and MODFLOW/MT3DMS-simulated *E. coli* concentrations. Simulation results indicated that groundwater and surface water systems affect *E. coli* transport in the subsurface; however, temporal variability of *E. coli* cannot be captured alone by groundwater and surface water integration.

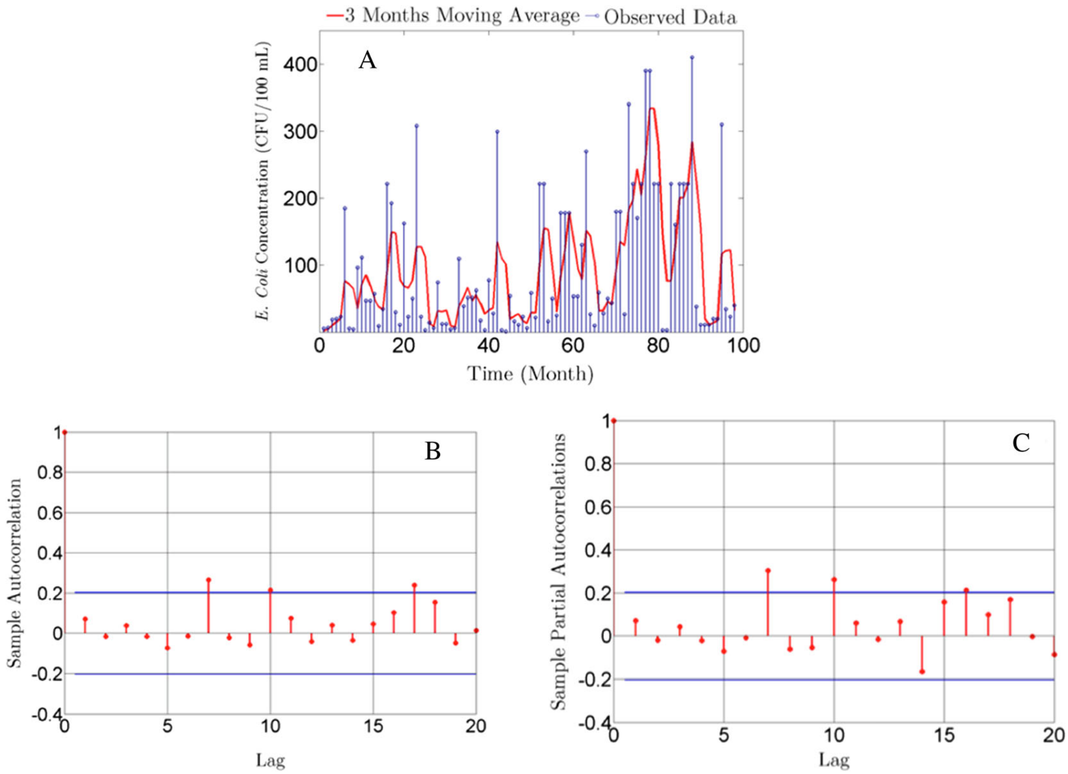

Fig. 3 The **a** 3-month moving average of *E. coli* concentrations (July 2002 to August 2010) in the monitoring station shows the seasonality in *E. coli* concentrations. The **b** autocorrelation (ACF) and **c** partial autocorrelation (PACF) functions of *E. coli* concentrations in the monitoring station describe the seasonality in the observed *E. coli* concentrations. The ACF and PACF demonstrate a repeating pattern of 7 and 10 months

Another set of simulation was carried out to consider SW-SoW-GW system (MODFLOW/MT3DMS and HYDRUS) so as to gain insight into the interpretation of processes controlling the *E. coli* transport in the subsurface. As suggested above, *E. coli* flux at the water table was calculated using HYDRUS and this flux served as the solute (contaminant) boundary condition for GW flow and transport (MODFLOW/MT3DMS). Simulated (using loosely coupled HYDRUS and MODFLOW/MT3DMS) and observed *E. coli* concentrations are shown in Fig. 4. Results show a reasonably good agreement between estimated and observed *E. coli* concentrations in the lake for calibration and validation periods. The NMSE value is 0.60 (calibration) to 0.55 (validation) from the simulated and observed *E. coli* concentrations. The uncertainty bands in Fig. 4 reflect the 95 % confidence interval of the model output. More than 85 % observed *E. coli* values fall within the confidence limits of $\pm\sigma$ (1 standard deviation). Nevertheless, 15 % *E. coli* values, which are not captured within $\pm\sigma$ interval, still fall within the 95 % confidence limits. Additionally, the mismatch between observed and estimated concentrations of *E. coli* can be a result of various sources of uncertainty. A key source of uncertainty—which is relatively difficult to incorporate—is related to the background concentrations of *E. coli* in soils and sediments (Pachepsky et al. 2006). Therefore, it is believed that as more data become available, these uncertainties will decline.

4.2 Effect of Seasonality on *E. coli* Transport

To better understand the impact of seasonality on *E. coli* transport in the subsurface, we consider two scenarios that incorporate GW table fluctuations in response to climatic conditions. Scenario 1 represents the hydrologic conditions in summer, where the water table is lower than the lake. Likewise, scenario 2 represents the hydrologic conditions in the winter, where the GW level is considered to be higher than the water level in the lake and canal. Consequently, GW gains water from the lake

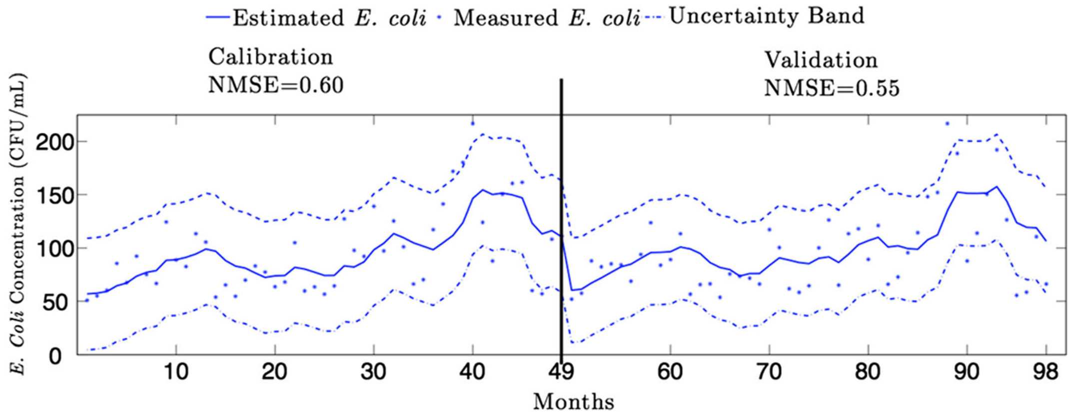

Fig. 4 Estimated *E. coli* concentrations from the calibrated MODFLOW/MT3DMS model and observed *E. coli* concentrations in the lake show that the observed *E. coli* values fall within the uncertainty band of 95 % confidence interval. Months from July 2002 to July 2006 (months 0–48 on the *X*-axis) and months from August 2006 to August 2010 (months 49–98) were used for calibration and validation, respectively

during summertime, and GW loses water to the lake during wintertime.

Figure 5 describes the characteristics of the *E. coli* breakthrough curves providing information on the peak concentrations of *E. coli* at observation nodes 1 and 2 (Fig. 1) for scenarios 1 (summer) and 2 (winter). It is evident from Fig. 5 that the peak concentrations of *E. coli* are smaller in the case of summer months as compared to winter months for both observation nodes 1 and 2. These results indicate less removal of *E. coli* in winter as compared to summer. In addition, Fig. 5 also demonstrates that higher peak concentrations of *E. coli* were obtained at observation node 2 than observation node 1 for both scenarios 1 (summer) and 2 (winter). This suggests that *E. coli* concentrations migrate toward the canal.

The *E. coli* concentration profiles in vertical and horizontal directions were examined to investigate the important characteristics of *E. coli* transport in the subsurface. Figure 6 shows the change in pressure head profiles during different scenarios (winter and summer). Figure 7 represents the concentration profiles of *E. coli* in the horizontal (1.5 m below land surface) and vertical directions along transect *A-A′* for scenarios 1 (summer) and 2 (winter). The lake and canal are located at 0 and 100 m, respectively, on the *X*-axis. Septic tanks are located at 15 and 85 m on the *X*-axis (Fig. 6). Figure 6a, c again

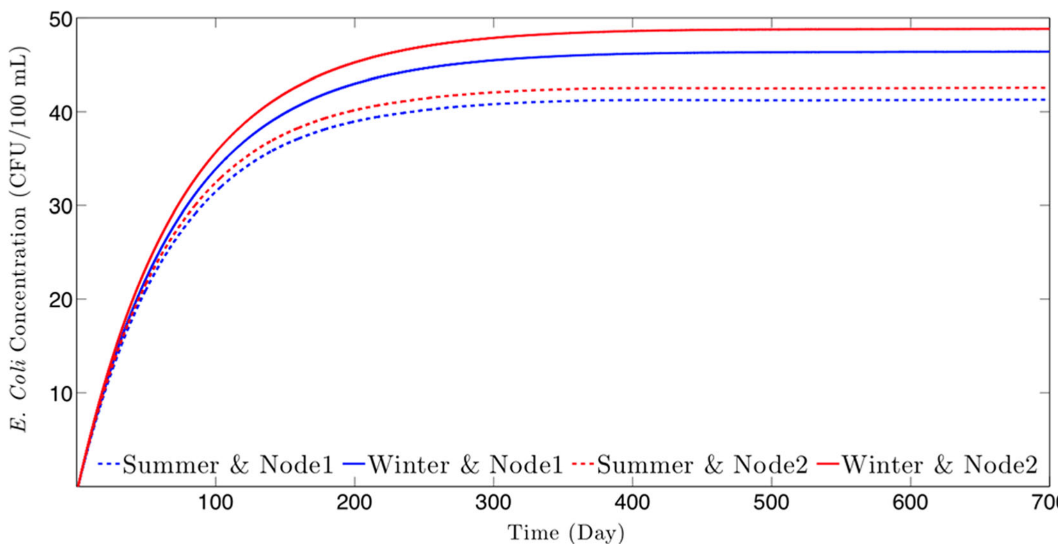

Fig. 5 The breakthrough curves of *E. coli* concentration at observation nodes 1 and 2 demonstrate the impact of scenarios 1 and 2 on *E. coli* transport in the subsurface. Scenario 1 represents summer, and scenario 2 represents winter

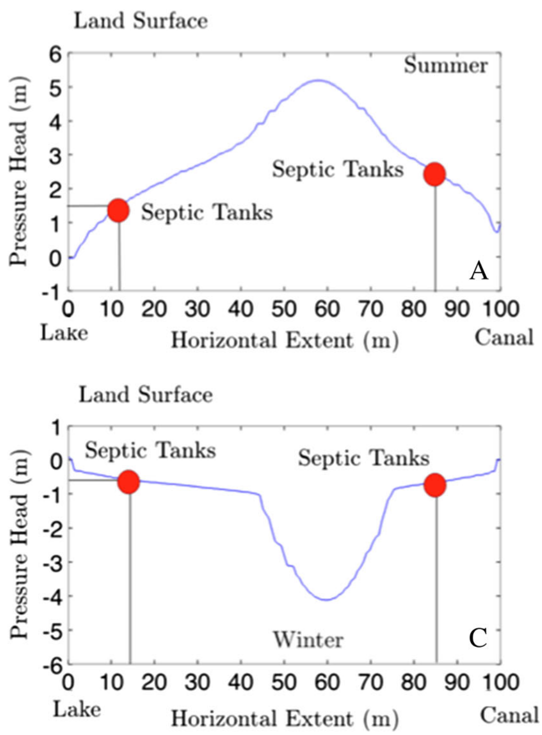

Fig. 6 The horizontal and vertical profiles (across septic tanks near the lake) of pressure head demonstrate the impacts of scenario 1 (summer)—**a** (horizontal profile) and **b** (vertical profile); and scenario 2 (winter)—**c** (horizontal profile) and **d** (vertical profile) on the extent of the saturated and unsaturated zones. Note that 5 m pressure head at 60 m lateral extent in **a** signifies pressure head obtained at depth below 5 m from the land surface (as shown in **b**)

demonstrates higher concentrations near the lake as well as the canal during winter times (scenario 2) as compared to summer times (scenario 1). As GW loses water during winter times (Fig. 5), there is advective transport toward the lake and canal from GW. Since the major transport modes of *E. coli* in the subsurface are through advective transport (Jamieson et al. 2003), higher *E. coli* concentrations were obtained at observation nodes 1 and 2 during winter times. In addition, wintertime (scenario 2) showed small fluctuations in *E. coli* concentrations near septic tanks (Fig. 7). These fluctuations may be attributed to infiltrating water because there is higher precipitation in the Lake Granbury area in the winter months. Figure 7 also depicts that *E. coli* concentration drops quickly toward the center of the modeling domain (42 to 58 m on the *X*-axis). This phenomenon—higher *E. coli* concentration near the lake and canal, and *E. coli* concentration dropping to zero toward the center of the modeling domain—shows that a GW divide exists in the modeling domain. The GW divide, defined by a hypothetical line on either side of which GW moves in opposite directions, occurs because of the shallow water table, which is strongly influenced by surface water flow (Anderson and Munter 1981). The GW divide prevents *E. coli* movement through advective transport toward the center of the modeling domain.

Figure 7b, d represents the concentration profile of *E. coli* in the vertical direction (by the septic tanks) for scenarios 1 (summer) and 2 (winter). Figure 7b, d manifests little upward retention of *E. coli* for both the scenarios. It is evident from this figure that the soil matrix within a depth of 0.5 m contains 90 % of *E. coli* from the source (septic tanks), which is consistent with previous studies (DeFlaun et al. 1997; Zhang et al. 2001; Jiang et al. 2007). In a column study, Tong et al. (2005) also reported that microbial deposition, under a variety of flow conditions and environmentally relevant ionic strength, decreases with distance from the source; however, deposition profiles have also been observed to exhibit a peak at some distance down gradient exhibiting sensitivity to system conditions.

Figure 7a–d further demonstrates that *E. coli* concentration gradually changes for scenario 2 (winter) than for scenario 1 (summer), wherein *E. coli* concentration drops quickly. In other words, scenario 2 (winter)

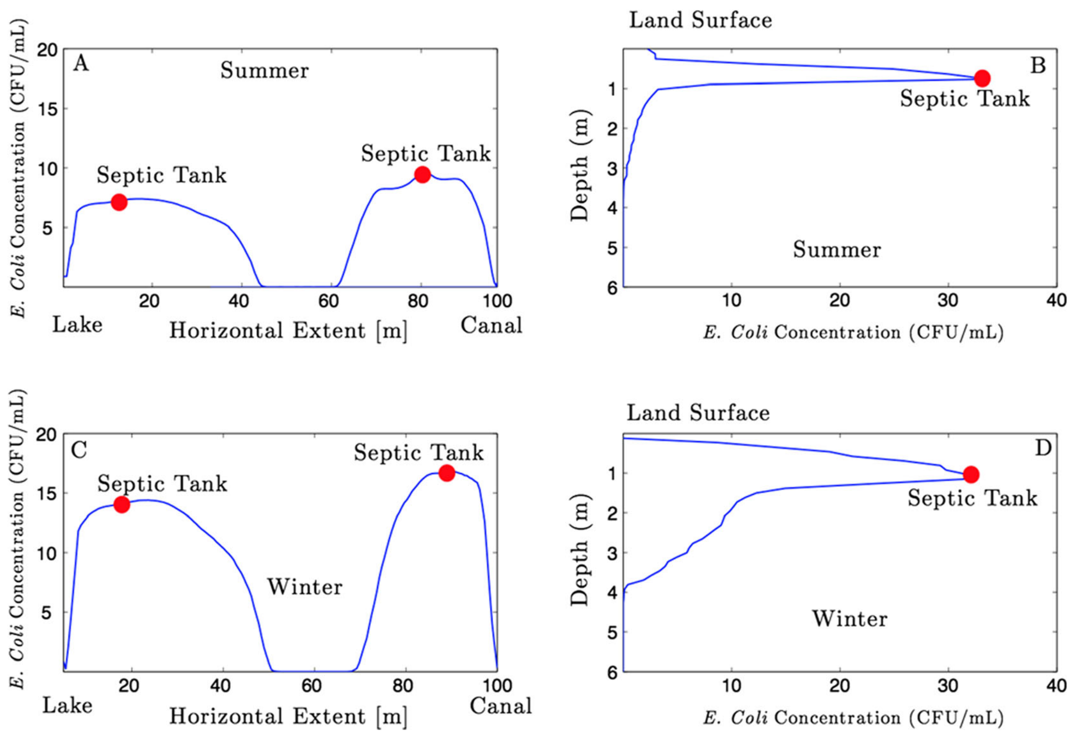

Fig. 7 The horizontal (1.5 m below land surface) and vertical profiles (across septic tanks near the lake) of *E. coli* concentration demonstrate the impacts of scenario 1 (summer)—**a** (horizontal profile) and **b** (vertical profile); and scenario 2 (winter)—**c** (horizontal profile) and **d** (vertical profile) on *E. coli* transport in the subsurface

displayed increased retained concentrations relative to scenario 1 (summer), possibly reflecting longer *E. coli* residence time for scenario 2 and, hence, greater attachment. These observations are also consistent with previous studies. For example, Tong et al. (2005) noted longer residence time for microbes in a sand column due to greater attachment caused by stagnant flow. Therefore, the gradual change in *E. coli* concentration for scenario 2 than for scenario 1 reflects that stagnant flow led to more attachment and longer residence times near the septic tanks toward the lake or canal. Hence, we conclude that these results demonstrate the importance of the flow regime and seasonal variability (climatic) on *E. coli* transport in the subsurface.

4.3 Sensitivity Analysis

It was found that the total retention rate coefficient was the most sensitive parameter followed by the saturated hydraulic conductivity. Similarly, in the unsaturated zone, the OFAT approach was implemented altering each parameter by ±30 % while keeping the rest of the parameters constant at their assigned values. It was found that *E. coli* concentration was largely affected by three parameters: saturated water content, total retention coefficient, and dispersivity.

Hydraulic conductivity is an important parameter for *E. coli* transport in the subsurface, and hydraulic conductivity is a function of soil water content in the unsaturated zone (van Genuchten 1980). Therefore, we notice that saturated water content and hydraulic conductivity are important parameters in the unsaturated zone and GW, respectively. The total retention rate coefficient is an important parameter for both the unsaturated zone and GW. These findings are congruous with previous studies found in the literature. For instance, a similar study, under variably saturated conditions, conducted by Long and Or (2007) reported diffusion as an important parameter for microbial deposition, which, in turn, is controlled by the soil water content. In addition, Or et al. (2007) demonstrated advective transport in the subsurface as the major mechanism for *E. coli* transport. Another study conducted by Powelson and Mills (2001) also demonstrated the impact of saturated water content and the retention rate on microbial transport and deposition.

5 Application of the Study Findings to Minimize Contamination of Water Resources

This study emphasizes the importance of flow paths and seasonal variability on *E. coli* transport in the subsurface. Our findings suggest that recharging and discharging hydrologic conditions strongly impact *E. coli* transport; these findings have significance for other environments with *E. coli* contamination. In real-world scenarios, the risk of contamination to water resources from *E. coli* can be minimized by correctly estimating the setback distance. Our study identifies the most sensitive parameters (e.g., hydraulic conductivity) with which a range of the setback distance under different conditions (e.g., soil type, temperature) can easily be estimated. For example, to objectively quantify the setback distance from septic tanks, *E. coli* inactivation or die-off rate is a key factor under variably saturated conditions. *E. coli* inactivation depends on various biotic and abiotic factors. The abiotic factors such as temperature, pore velocity, and oxygen show large variability in times ranging from hours, days, months, to seasons (Logan et al. 1995; Saiers 2005; Foppen and Schijven 2006). Other abiotic factors, such as grain size, porosity, and soil type, show large spatial variability from pore to field scales (Tufenkji et al. 2004; Tufenkji 2007). We must note that *E. coli* movement in the subsurface under variably saturated conditions may range from submeter to a few meters. Data on these factors may not be available in different field conditions at present; however, we can estimate a range of the setback distance by perturbing the most sensitive parameters (e.g., saturated water content of the soil, total retention rate coefficient, hydraulic conductivity). Additionally, optimal monitoring locations can also be designed to enable informed decisions for safeguarding water resources across the world.

6 Limitations and Scope of the Study

To appropriately describe the fate and transport of *E. coli* at the field scale, it is important to determine the level of complexity needed in the modeling framework. Currently, it is not possible to incorporate the effect of various biotic (grazing, competition posed by protozoa) and abiotic (e.g., temperature, pore velocity, oxygen) factors in the modeling framework at the field scale due to unavailability of observations, difficulty in measurements, and inherent stochasticity in these factors. For keeping up with the goal of this study, which was to evaluate *E. coli* transport in the subsurface zone under recharging-discharging GW, *E. coli* inactivation or die-off was simplified and represented by the total retention rate coefficient. We believe that our conceptual model for describing the *E. coli* transport in SW-SoW-GW represents the adequate complexity and is, therefore, robust to this simplification. However, it is desirable to include more complexity in the modeling framework in future studies to minimize uncertainty in *E. coli* estimation, which may be possible through the availability of more data in the future.

7 Conclusions

A major goal of this research was to investigate *E. coli* transport in the subsurface by considering saturated zone processes only and then by linking the surface water-soil water-groundwater system. Two hydrologic scenarios based on expected water level variations in the lake and canal were implemented to investigate seasonal controls on *E. coli* transport in the subsurface in the Lake Granbury area. The loosely coupled HYDRUS and MODFLOW/MT3DMS models were able to produce a reasonably good agreement between the estimated and observed *E. coli* concentrations in the lake. Results indicate that although groundwater and surface water system largely control *E. coli* transport in the subsurface, temporal variability of *E. coli* can be described by linking the SW-SoW-GW system. Results further show slightly less removal of *E. coli* in recharging GW months as compared to discharging GW months. It was found that 90 % *E. coli* are retained in the soil matrix within a depth of 0.5 m from the source (septic tanks). Water content, total retention rate coefficient, and hydraulic conductivity are important parameters for describing *E. coli* transport in the subsurface. The flow paths in the Lake Granbury area indicate that the canal is more at risk of impairment than the lake. However, if this condition persists, in time, the main body of the lake will also be at risk. These results are useful to decision makers and environmental managers to design targeted monitoring programs by incorporating seasonality and supporting real-time decision-making.

Acknowledgments This research was supported by EPA 319(h) grant for TMDL in Texas streams and partly supported by the National Institute of Environmental Health Sciences (grant 5R01ES015634), Texas Water Resources Institute, and Texas A&M support a/c 02-130003. The content is solely the responsibility of the authors and does not necessarily represent the official views of the funding agencies.

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