MaSTiS, Microorganism and Solute Transport in Streams

Model Documentation and User Manual

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December, 2013

Abstract

In-stream fate and transport of solutes and microorganisms need to be understood to evaluate its suitability for agricultural, recreational, and household uses. e. Concerns of safety of this water resulted in development of predictive models for estimating concentrations and total numbers of pathogen and/or indicator organisms being released during and after high-water flow events. The purpose of this technical bulletin is to describe the MaSTiS (**M**icroorganism **a**nd **S**olute **T**ransport in **S**treams) mathematical model and the corresponding computer code. Transport of microorganisms and solutes are simulated based on advection-dispersion equations coupled with the Saint-Venant equations that model flow of surface stream water. The models accounts for the transient storage effect. Input and output files are described and examples are provided.

Disclaimer

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Note on Units

The generic symbol NoM (is used throughout the manual and in input and output files to represent the amount of microbes. Depending on the microorganism and microbiological analysis method, NoM may mean number of cells, MPN (Most Probable Number), CFU (colony forming units), PFU (plague forming units), cysts, etc.

List of symbols

A	creek cross-sectional area, m^{2}
A_{st}	cross-sectional area of the transient storage zone, m^{2}
C	microbial concentration in stream, NoM m^{-3}
C_b	microbial concentration in streambed sediments, NoM kg^{-1}
C_g	microbial concentration in groundwater, NoM m^{-3}
C_{st}	microbial concentration in transient storage, NoM m^{-3}
c_d	drag coefficient
D	dispersion coefficient, m^{2} s^{-1}
f_{st}	storage ratio parameter
g	gravitational acceleration, m s^{-2}
h	height of water column (m)
H_b	streambed layer of a thickness, m
k_{dw}	bacteria die-off rate in water, s^{-1}
k_{ds}	bacteria die-off/production rate in sediments, s^{-1}
M	mass unit, e.g. g, mg, etc.
n	bed roughness
Q	stream discharge, m^{3} s^{-1}
q_{g}	groundwater flux (upwelling) to the creek per unit of creek length, m^{2} s^{-1}
R_e	entrainment coefficient, kg m^{-2}s^{-1}

R_d	microbial deposition rate, m s^{-1}
R_r	microbial resuspension rate, kg m^{-2} s^{-1}
S_F	friction slope
S_0	bed slope
t	time (s),
u	average flow velocity (m s^{-1}),
v_s	settling velocity, m s^{-1}
w	creek width, m
x	distance along creek (m)
α	stream-storage exchange coefficient, s^{-1}
ρ_b	sediment bulk density, kg m^{-3}
τ_b	bed shear stress, N m^{-2}
τ_{cr}	critical shear stresses for resuspension, N m^{-2}
τ_{cd}	critical shear stresses for deposition, N m^{-2}

1. Introduction

Microbial activity influences the safety of use of surface waters for recreation, irrigation, aquaculture, husbandry, as well as for drinking and household needs. Fecal bacteria like entererocci and *Escherichia coli* are commonly used to evaluate the sanitary quality of water and their high numbers suggest an increased likelihood of presence of bacterial pathogens which can adversely impact human health (Wade et al., 2006). *E. coli* is the leading indicator of microbial contamination of natural waters (US EPA, 2003). There is a need to understand in-stream fate and transport of *E. coli* so as to understand and limit contamination of surface water by microbial organisms.

The existing frameworks for modeling bacteria transport in steams are based on advection-dispersion transport and sediment–water column interactions. Currently, models of sediment/bacteria transport in streams account for processes of resuspension and settling (Steets and Holden, 2003; Jamieson et al., 2005; Bai and Lung, 2005; Cho et al., 2010, Russo et al., 2011, etc). However, these models disregard the effect of transient storage (TS), i.e. dead-end zones represented by stagnant pools, eddies etc. (Bencala and Walters, 1983, Gooseff et al., 2008). Neglecting TS does not allow one to simulate long tails observed on the graphs of *E. coli* concentrations as a function of time or cumulative water discharge. Models with a term for TS need to be developed and evaluated for better understanding the release and transport of bacteria in streams (Yakirevich at al., 2013). The purpose of this technical bulletin is to describe the MaSTiS (**M**icroorganism **a**nd **S**olute **T**ransport **i**n a **S**tream) mathematical l model and the corresponding computer code.

Transport of microorganisms and solutes is simulated based on advection-dispersion equations coupled with the Saint-Venant equations modeling flow of stream water.

This bulletin includes:

1. Brief description of the mathematical models for the processes involved,
2. Description of the program structure and the data requirements for microorganism transport simulation,
3. Examples to help users to better understand the model inputs and generated output information.

2. Theory

A one-dimensional model is applied to simulate water flow, microorganisms and conservative tracer transport during transient flow in a creek/canal.

2.1. Flow model

The shallow water Saint–Venant equations were used to calculate water depth and discharge. The continuity and the momentum equations, respectively, are (Cunge et al., 1980):

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_g \qquad (1)$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{Q^2}{A} + gI_1\right) = gA(S_0 - S_F) + gI_2 + \beta q_g u \qquad (2)$$

where *A* is the cross-sectional area (m^2), *Q* is the discharge (m^3 s^{-1}), q_g is the groundwater flux to the creek per unit of creek length, (m^2 s^{-1}), $S_F = n^2 u|u|/h^{4/3}$ is the friction slope (–), *n* is the bed roughness, S_0 is the bed slope (–), g = 9.8 is the acceleration of gravity (m s^{-2}), $u=Q/A$ is the average flow velocity (m s^{-1}), $\beta \approx 1$ accounts for the effect of groundwater upwelling on momentum of flow, *x* is the distance along creek (m), and *t* is time (s), *h* is the height of water column (m)

$$I_1 = \int_0^h (h-z) w(x,z)\, dz \text{ and } I_2 = \int_0^h (h-z) \frac{\partial w(x,z)}{\partial x} dz \tag{3}$$

where and *w* is the creek width.

For the simplicity we consider a stream of a rectangular cross-section of the width *W*(*x*), then

$$I_1 = Ah/2\,,\; I_2 = bh^2/2 \tag{4}$$

where $b = \partial W/\partial x$.

2.2. Model of in-stream transport of microorganisms and conservative solutes

. The one-dimensional stream solute transport model accounts for advection-dispersion, lateral inflow/outflow, exchange with TS, linear die-off/production, and resuspension of bacteria from bottom sediments. We consider only one type of microorganism in the water column and in the sediment, and their resuspension from bed sediments and settling is characterized by lumped parameters that can be estimated based on experimental data.

The governing equation of stream microbial transport has a form

$$\frac{\partial (AC)}{\partial t} = \frac{\partial}{\partial x}\left(AD \frac{\partial C}{\partial x} \right) - \frac{\partial (QC)}{\partial x} - \alpha A (C - C_{st}) + q_g^+ C_g - q_g^- C + WR_r C_b - WR_d C - k_{dw} AC \tag{5}$$

where C and C_{st} are the *E. coli* concentration in stream and TS, respectively (NoM m^{-3} or M m^{-3}), D is the dispersion coefficient ($m^2\ s^{-1}$), α is stream-storage exchange coefficient (s^{-1}), R_r and R_d are microorganism resuspension (kg $m^{-2}\ s^{-1}$) and deposition rates (m s^{-1}), respectively, C_b is the microorganism concentration in streambed sediments (NoM kg^{-1}), C_g is the microorganism concentration in groundwater (NoM m^{-3}), $q_g^{\pm} = \left(q_g \pm \left|q_g\right|\right)/2$, and k_{dw} is the bacteria die-off rate in water (s^{-1}).

Exchange with TSis governed by a linear kinetic equation assuming first-order mass transfer (Bencala and Walters, 1983)

$$\frac{\partial\left(A_{st}C_{st}\right)}{\partial t} = \alpha A\left(C - C_{st}\right) - k_{dw}A_{st}C_{st} - hv_s C_{st} \tag{6}$$

where A_{st} is cross-sectional area of the TS zone (m^2), and v_s is the settling velocity (m s^{-1}). Note that we neglect the bacteria release in TS zone. Since both the stream and the storage zone cross-sectional areas vary with time, a dimensionless measure of the storage effect is obtained by calculating the ratio of storage zone cross-sectional area to main channel cross-sectional area (Runkel et al., 1999). We assume that the storage ratio parameter, $f_{st} = A_{st}/A$, does not change with time, yet, it is stream reach-specific.

The microorganism mass balance equation in a streambed layer of a thickness H_b is

$$H_b\rho_b \frac{\partial C_b}{\partial t} = -R_r C_b + R_d C - k_{ds}H_b\rho_b C_b \tag{7}$$

where k_{ds} is the bacteria die-off/production rate in sediments (s^{-1}), and is ρ_b the sediment bulk density (kg m^{-3}).

The resuspension and deposition rates are calculated as (Russo et al., 2011):

$$R_r = \begin{cases} R_e\left(\tau_b/\tau_{cr} - 1\right) & \text{for } \tau_b > \tau_{cr} \\ 0 \quad \text{for } \tau_b \le \tau_{cr} \end{cases} \tag{8a}$$

$$R_d = \begin{cases} v_s\left(1 - \tau_b/\tau_{cd}\right) & \text{for } \tau_b < \tau_{cd} \\ 0 \quad \text{for } \tau_b \ge \tau_{cd} \end{cases} \tag{8b}$$

where R_e is the entrainment coefficient (kg m^{-2}s^{-1}), τ_b is the bed shear stress (N m^{-2}), v_s is the settling velocity (m s^{-1}), τ_{cr} and τ_{cd} are critical shear stresses for resuspension and deposition, respectively (N m^{-2}). The critical shear stress for deposition is set as $\tau_{cd} = 0.8\tau_{cr}$, based on data of Russo et al. (2011).

A fairly good approximation of the average shear stress at the bed can be also obtained using the quadratic stress law, which relates stress to the square of the average fluid velocity (u) (Schlichting, 1987)

$$\tau_b = \rho c_d u^2 \tag{9}$$

where ρ is water density (kg m^3), and c_d is the drag coefficient (-). In our simulations we use average value of c_d=0.003 (Cardenas et al., 1995).

The longitudinal dispersion is expected to increase with increasing discharge and flow velocity (Wallis and Manson, 2004), due to turbulence structures developing within the water column. We assume a linear dependence of the dispersion coefficient on flow velocity, as commonly accepted in porous media transport simulations (Bear, 1979), i.e. $D=a_L u$, where a_L is the longitudinal dispersivity (m).

To describe transport of a conservative tracer in a stream, we use equations (5) and (6) assuming zero die-off/production rate, and negligible resuspension-deposition processes.

2. 3. Initial conditions boundary conditions and numerical solution

For the Saint-Venant equations, the initial conditions define the distribution of water fluxes and water depth along the creek at t=0; while boundary conditions specify the value of flux as a function of time at the stream inlet (for the supercritical flow, also the value of water depth is prescribed), and the transmissive boundary at the outlet. For the transport equation, the initial conditions define the concentration of microorganism or conservative tracer in water and bottom sediment layer along the creek at t=0; while boundary conditions specify value of concentration in water column as a function of time at the stream inlet, and the zero dispersive flux (the Neumann boundary condition) at the outlet.

The Saint-Venant equations were solved numerically by the finite volume (FV) method using a central-upwind scheme (Kurganov and Petrova, 2008) and the fourth order Runge-Kutta method with the estimate of truncation error (England, 1996) and the adaptive step size control (Press et al., 1989). The transport equations were solved by using implicit finite differences (FD) method and applying the front limitation algorithm (Haefner et al., 1997). The FORTRAN code was developed to implement the numerical algorithm. Benchmarking was performed using the dam break solution (Stoker, 1957) for the Saint-Venant equations, and analytical solutions for the advection dispersion equation (Van Genuchten and Alves, 1982).

A uniform FD grid is introduced to solve transport equations. The grid step size:

$$h_x = L/(N_{fdn} - 1) \tag{10}$$

where L is simulated stream length (m) and N_{fdn} is the number of nodes in the FD grid. The nodes of the FV mesh are located at the middle of the FD grid elements.

The total length of the stream is subdivided into segments (reaches). Stream parameters (e.g., slope, roughness, transport parameters, initial conditions, etc.) in each segment have constant values. Segments can be different for different parameters. Total simulation time is also subdivided by time intervals.

3. MaSTiS program documentation

3.1. Program structure description

A FORTRAN code has been written to implement the MaSTiS model. The code is structured with subroutines, each performing specific functions listed in Table 1.

Table 1. MaSTiS subroutines

Subroutines	Functions
MaSTiS	Main program
CrMicINP	Data input
CrMicGrid	Constructing FV mesh & FD grid
INTERP1	Interpolating parameters and initial conditions into grids
CrMicStor	Calculating water volume and solute mass in the domain
ODEINT_E	Adaptive stepsize control for solving ODE by Runge-Kutta method (taken from Numerical Recipies by Press et al., 1992)
RKQC_ENG	Forth-order Runge-Kutta-England step with monitoring of local trancation error (modified from Numerical Recipies by Press et al., 1992)
STWICSV	Solving transport equation at each time step
TSYSO	Solving set of linear equations with 3-diaganal matrix by the Thomas algorithm with pivoting
RK4_ENG	One time step to solve ODE by the Runge-Kutta-England method
RHS_SV	Calculates Right Hand Side (time derivatives dU/dt=RHS) of the Saint-Venant equations
PWLRec	Peace-Wise Linear REConstruction of a function U in a FV cell
FMINMOD3	Calculates MinMod of 3 variables

3.2. Input data

The code does not check correctness of data in files. Values of variables and parameters are separated by one or few spaces. Except the text information, data values are introduced either as an INTEGER number that has no fractional part and no decimal point; or a REAL as a signed number with a decimal point and the exponent (e.g, *±0.mE±p* for very small or very large values if required). Following input files are required to run MaSTiS code: **crparam.txt** (stream parameters) and **crbicond.txt** (initial and boundary conditions, and output info).

Structure and description of input variables for the **crparam.txt** file are presented in Tables 1 and 2, respectively. All data are subdivided by several groups

Table 1: Structure of the input file **crparam.txt**

Group #, number of rows, Type of data	**Description**
1, 1, text	Simulated problem title (up to 80 symbols)
2, 1, text	NTR Ninv Nfdn
2, 1, INTEGER	Values of NTR, Ninv, Nfdn
3, 1, text	L BTm0
3, 1, REAL	Values of L, BTm0
4, 1, text	NWidth
4, 1, INTEGER	Value of NWidth
4, 1, text	XWidth Width
4, Nwidth, REAL	Values of XWidth, Width (2 numbers in each row)
5, 1, text	Nslope
5, 1, INTEGER	Value of Nslope
5, 1, text	XSl Slope
5, Nslope, REAL	Values of XSl Slope (2 numbers in each row)
6, 1, text	NRough
6, 1, INTEGER	Value of NRough
6, 1, text	XRough Rough
6, NRough, REAL	Values of XRough Rough (2 numbers in each row)
7, 1, text	NGWUp
7, 1, INTEGER	Value of NGWUp
7, 1, text	XGWU QGWU CGWU
7, NGWUp, REAL	Values of XGWU QGWU CGWU (3 numbers in each row)
	Group 8 is needed if NTR=1 only (for transport simulations)
8, 1, text	NTrPar
8, 1, INTEGER	Value of NTrPar
8, 1, text	XTr aL Re TAUCR f Vs Alfa Kdw Kds TSS Hb Rb
8, NTrPar, REAL	Values of XTr aL Re TAUCR f Vs Alfa Kdw Kds TSS Hb Rb

Table 2: Description of data in the input file **crparam.txt**

Group	Data	Description
2	NTR	Microbial/solute Transport flag.(0-not solved, 1-solved)
	Ninv	0-Dummy parameter
	Nfdn	Number of nodes in FD grid (max 1000)
3	L	Stream length (m)
	BTm0	Bottom elevation at X=0 above some reference level, (m)
4	NWidth	Number of stream segments +1 with different width (max 100)
	XWidth	Coordinate of starting point for each segment (last segment ends at X=L)
	Width	Stream width (*w*)of a segment, m
5	Nslope	Number of stream segments plus +1 with different bed slope (max 100)
	XSl	Coordinate of starting point for each segment (last segment ends at X=L)
	Slope	Streambed slope (S_0) of a segment
6	NRough	Number of stream segments +1 with different bed roughness (max 100)
	XRough	Coordinate of starting point for each segment (last segment ends at X=L)
	Rough	Streambed roughness (n) of a segment
7	NGWUp	Number of stream segments +1 with different upwelling (max 100)
	XGWU	Coordinate of starting point for each segment (last segment ends at X=L)
	QGWU	groundwater upwelling (q_g) to the creek per unit of creek length, m^2 s^{-1}
	CGWU	Microbial/solute concentration in groundwater, NoM m^{-3}
8	NTrPar	Number of stream segments +1 with different transport param. (max 100)
	XTr	Coordinate of starting point for each segment (last segment ends at X=L)
	aL	Longitudinal dispersivity (a_L), m
	Re	Microbial entrainment rate (R_e), kg m^{-2} s^{-1}
	TAUCR	Critical shear stresses for resuspension (τ_{cr}), N m^{-2}
	f	Storage ratio parameter (f_{st})
	Vs	Settling velocity (v_s), m s^{-1}
	Alfa	Stream-storage exchange coefficient(α), s^{-1}
	Kdw	Sacteria die-off rate (k_{dw}) in water, s^{-1}
	Kds	Sacteria die-off/production rate (k_{ds}) in sediments, s^{-1}
	TSS	Total suspended solids, kg/m^3 – not used
	Hb	Streambed mixing layer thickness (H_b)
	Rb	Sediment bulk density (ρ_b), t m^{-3} (need to check)

*

Structure and description of input variables for the **crbicond.txt** file are presented in Tables 3 and 4, respectively. All data are subdivided by several groups

Table 3: Structure of the input file **crbicond.txt**

Group #, number of rows, Type of data	**Description**
1, 1, text	NInCW
1, 1, INTEGER	Value of NInCW
1, 1, text	XInCW hIni QIni
1, NInCW, REAL	Values of XInCW hIn Qin (3 numbers in a row)
	Group 2 is needed if NTR=1 only (for transport simulations)
2, 1, text	NInCT
2, 1, INTEGER	Value of NInCT
2, 1, text	XInCT CwIni CsIni
2, NInCW, REAL	Values of XInCT CwIn CsIn (3 numbers in a row)
3, 1, text	NTI NB0 NBL
3, 1, INTEGER	Value of NTI 1 1
3, 1, text	TBC hb0 Qb0 CB0
3, NTI, REAL	Values of TBC hb0 Qb0 CB0 (4 numbers in a row)
4, 1, text	NTOUT
4, 1, INTEGER	Value of NTOUT
4, 1, text	TOUT (1,...NTOUT)
4, 1, REAL	Values of TOUT
5, 1, text	Nobs
5, 1, INTEGER	Value of Nobs
5, 1, text	XObs (1,...Nobs)
5, 1, REAL	Values of XObs

Table 3: Description of data in the input file **crbicond.txt**

Group	Data	Description
1	NInCW	Number of points to prescribe initial conditions for flow (max 1000)
	XInCW	Coordinate where the initial conditions prescribed, m
	hIni	Initial water elevation value in stream, m
	QIni	Initial water discharge value in stream, m^3 s^{-1}
2	NInCT	Number of points to prescribe initial conditions for flow (max 1000)
	XInCT	Coordinate where the initial conditions prescribed, m
	CwIni	Initial bacteria/solute concentration in water, NoM m^{-3} or g m^{-3}
	CsIni	Initial bacteria/solute concentration in bed sediments, NoM t^{-3} or M t^{-3}
3	NTI	Number of time intervals with different boundary condition (max 1000)
	NB0	Type of boundary condition at the inlet NB0=1
	NBL	Type of boundary condition at the outlet NBL=1
	TBC	End of the time interval, sec
	hb0	Water elevation at the inlet boundary
	Qb0	Water discharge at the inlet boundary, m^3 s^{-1}
	CB0	Concentration at the inlet boundary, NoM t^{-3} or M t^{-3}
4	NTOUT	Number of times for output info along stream in each FD node (max 100)
	TOUT	Times for output info along stream in each FD node
5	Nobs	Number of observation stations/nodes (max 10)
	Xobs	Coordinates of observation stations/nodes

3.3. Output files

The MaSTiS code creates two output files: **crOutput.txt** and **crObsNode.txt**. The **crOutput.txt** file contains all input information and results of simulations at times TOUT. These results include the table of calculated values of water elevation h (m), flow velocity u (m/s), discharge per unit width $q=uh$ (m^2/s), total water discharge Q (m^3/s), concentration in water C (NoM m^{-3} or M m^{-3}), concentration in bed sediments C_b (NoM t^{-3} or M t^{-1}), and concentration in transient storage water C_{st} (NoM m^{-3} or M m^{-3}) at each FV node. The table of variables distribution along the steam is followed by the tables of water and solute balances in water and sediments.

The **crObsNode.txt** file contains calculated values of water elevation h (m), flow velocity u (m/s), total water discharge Q (m^3/s), concentration in water C (NoM m^{-3} or M m^{-3}), concentration in bed sediments C_b (NoM t^{-3} or M t^{-1}) at observation stations/nodes for approximately every 60 sec of simulated time.

3.4. Running the code

The MaSTiS runs by clicking twice the executable file MaSTiS.exe. The input files must be located and the output files are created at the same folder. Progress of simulations is shown on a the monitor for every 60 sec of simulation time.

The code was compiled with the following versions of FORTRAN: PowerStation 4.0, Compaq 6.0, and Intel® Visual Fortran Composer XE for Windows. All executable codes produce similar results.

4. Example problems

The example problems demonstrating the MaSTiS code application are presented in this section. In this example the model reproduces the results of *E. coli* release and transport from bottom sediment and a conservative tracer DFBA transport in a creek during the artificial high-water flow events in July 2009 (Yakirevich et. al, 2013).

4.1 Description of study area and the experiment

The study site (Figure 1) is located at the Optimizing Production Inputs for Economic and Environmental Enhancement (OPE3) watershed research site, USDA-Beltsville Agricultural Research Center on the mid-Atlantic coastal plain of Maryland. The site contains a small first-order creek (the Beaver Dam Creek Tributary described in detail by Angier et al., 2005) of ~1100 m long that is instrumented with four stations for monitoring stream flow and water sampling. The creek bed is from 100 to 160 cm wide and bed slope varies along the creek from

0.0008 to 0.0122 (Cho et al., 2010). The creek runs within a riparian corridor of variable width from about 65 m at its narrowest point, to more than 100 m. Four fields (A, B, C, and D in Figure 1, total area of 22.5 ha) have been under continuous corn production for the last 12 years. Field A receives 70,000 kg ha^{-1} dairy manure annually, whereas other fields receive only chemical fertilizers. Mean electrical conductivity and pH of water measured before and during experiment were 136±58.2 µS cm^{-1} and 6.91±0.35, respectively.

Four sampling stations located at 10, 150, 290 and 640 m from the water release point were instrumented with weirs and automated refrigerated samplers (Sigma 900 Max All Weather Refrigerated Sampler, Hach Company, Loveland, CO) to measure depth of water and to sample water in the creek (Figure 1). The weirs have been calibrated to convert depth of water to flow rate (Hively et al., 2006). The sections of the creek between stations 1 and 2, 2 and 3, and 3 and 4 are referred below as reach 12 (~140 m length), reach 23 (~140 m length), and reach 34 (~350 m length), respectively. The Trimble GeoXM 2005 Series global positioning system was used to determine elevations of the creek bottom at incremental distances along the creek. Creek sediment was sampled at 20-m increments along the creek to measure particle size distribution in the top 1-cm layer of the streambed. Fifty grams of sediment were collected at four positions across the creek at each sampling location to represent the texture variation across the stream.

The artificial high-flow experiment was conducted on July 21, 2009. The creek sediment was sampled for *E. coli* concentrations equidistantly (every 20 m) in four replications within each reach 1 h before and one day after the high-flow event. Composite samples were taken across the creek from the top 2-cm layer of the streambed. The artificial high-flow event was created by releasing city water on a tarp-covered stream bank 10 m upstream from station 1 at a rate of around 60 L s^{-1} in four allotments of 11.0, 17.9, 11.5, and, 16.0 m^{3}. A conservative tracer difluorobenzoic acid (DFBA) was added to the release water at concentrations of 31.5, 0.6, 0.16, and 0.0 ppm in each allotment, respectively. Water was delivered in trucks, and time intervals between allotments (1 min, 3 min, and 1 min) were determined by truck logistics.

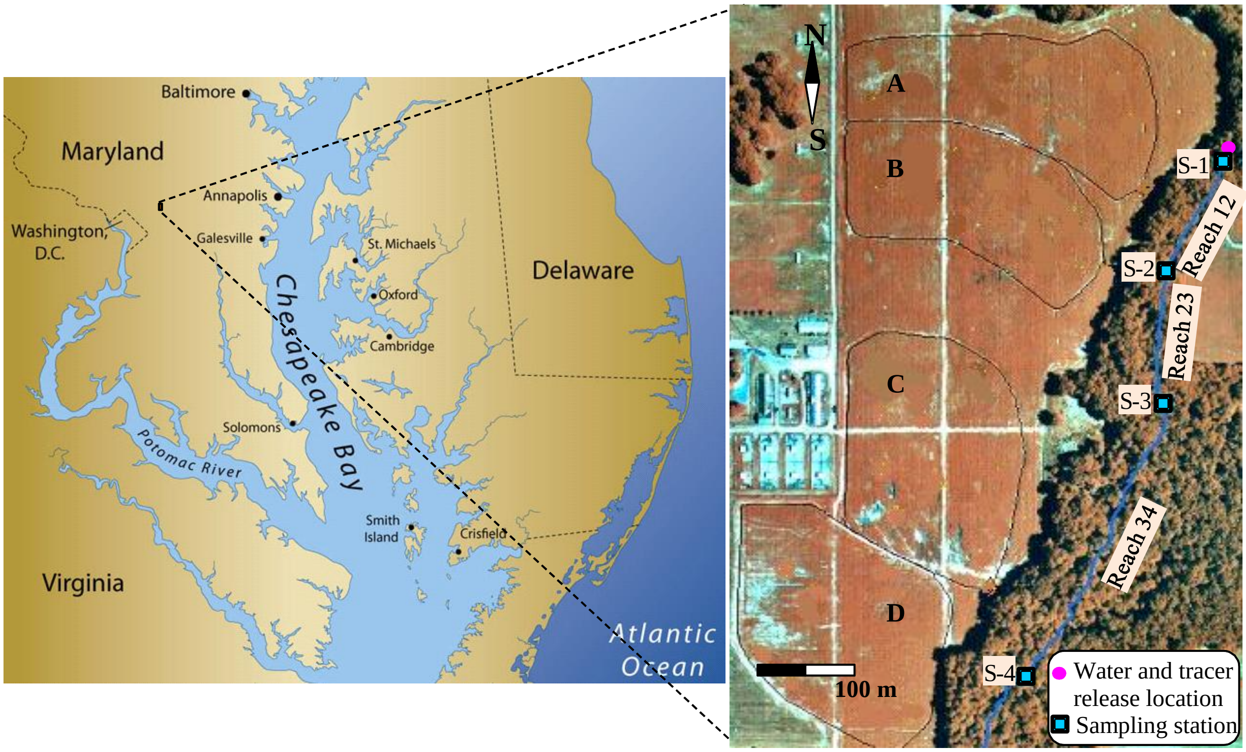

Figure 1. Study area at the USDA-ARS the OPE3 research site.

4.2 Simulation results

Analysis of Beaver Dam Creek data relied on the trial-and-error approach. Reach-specific model parameters were estimated manually by using observed time series of water flow rates and concentrations of *E. coli* and the conservative tracer DFBA at stations 2, 3 and 4. Any groundwater upwelling flux into the creek was calculated for each section of the creek between the weirs based on water balance as a difference between discharge at the reach outlet and inlet per unit length. Firstly, flow parameters were estimated by fitting simulated arrival time of artificially induced wave to the observed arrival time at a reach outlet. The bed roughness parameter (*n*) was changed consequently for each reach to fit the model simulations and observation. The second step was to estimate transport parameters: dispersivity (*a*), storage ratio (f_{st}) and exchange rate parameter (α) for each reach using DFBA breakthrough curves (BTCs). Calibration started from reach 12 by changing above three parameters for this reach, while holding values (initial guess) of these parameters at downstream reaches constant. When satisfactory agreement between observed and simulated BTCs at station 2 was achieved, this stepwise procedure was performed for each of the downstream reaches. Third step was to estimate parameters of bacteria resuspension using *E. coli* BTCs at stations 2, 3, and 4: the entrainment coefficient (R_e) and the critical shear stresses for resuspension (τ_{cr}). If a reasonable fit of *E. coli* BTCs was not achieved for the tested range of resuspension parameters values, then additional trial simulations were performed by modifying the storage ratio and exchange rate parameters initially found from DFBA tracer simulations.

Simulated length of the stream was chosen as L=650 m from the inlet till a point located 10 m behind the station 4. Number of nodes in the FD grid was equal 261, i.e. FD stepsize is 2.5 m. The initial values of the water level and the water discharge were known at the 4 points only, as measured at the stations. Therefore, in first simulations for DFBA transport, we prescribe these boundary conditions and run the simulation for 2000 sec with boundary condition at the inlet using measured values of water level and discharge at the inlet before the experiment started. This allows to establish steady flow and obtain values of water level and discharge in all grid nodes to be used in simulations for *E. coli* transport.

Table 1 to 3 shows the parameters associated with the flow and transport model along with model goodness-of-fit indices.

Table 1 Estimated flow model parameters and goodness of fit indexes for the Beaver Dam Creek Tributary in 2009

Reach	12	23	34
Groundwater flux, q_{gw}x10^6 m^2 s^{-1}	15.7	6.37	1.15
Manning's roughness, n	0.14	0.06	0.08
Nash-Satcliffe efficiency, NSE	0.625	0.774	0.599
Modified index of agreement, MIA	0.823	0.887	0.805

Table 2 Estimated parameters of DFBA tracer transport and goodness of fit indexes for the Beaver Dam Creek Tributary in 2009

Reach	12	23	34
Dispersivity, a, m	0.9	0.7	0.5
Transient storage ratio, $f_{st}=A_{st}/A$	0.2	0.2	0.1
Exchange rate, α x10^4, s^{-1}	4.0	2.0	1.0
Nash-Satcliffe efficiency, *NSE*	0.813	0.839	0.477
Modified index of agreement, *MIA*	0.905	0.915	0.730

Table 3 Estimated *E. coli* transport parameters and goodness of fit indexes for the Beaver Dam Creek Tributary in 2009

Reach	12	23	34
Transient storage ratio, $f_{st}=A_{st}/A$	0.3	0.5	0.4
Exchange rate, α x10^4, s^{-1}	7.0	5.0	3.0
Critical shear stress, τ_{cr} , N m^{-2}	0.02	0.03	0.02
Entrainment rate, R_e x10^3, kg m^{-2}s^{-1}	65.0	23.0	4.0
Nash-Satcliffe efficiency, *NSE*	0.594	0.327	0.443
Modified index of agreement, *MIA*	0.817	0.667	0.722

Figure 2 shows results of simulations for the discharge, tracer and concentrations along with observed data at three stations.

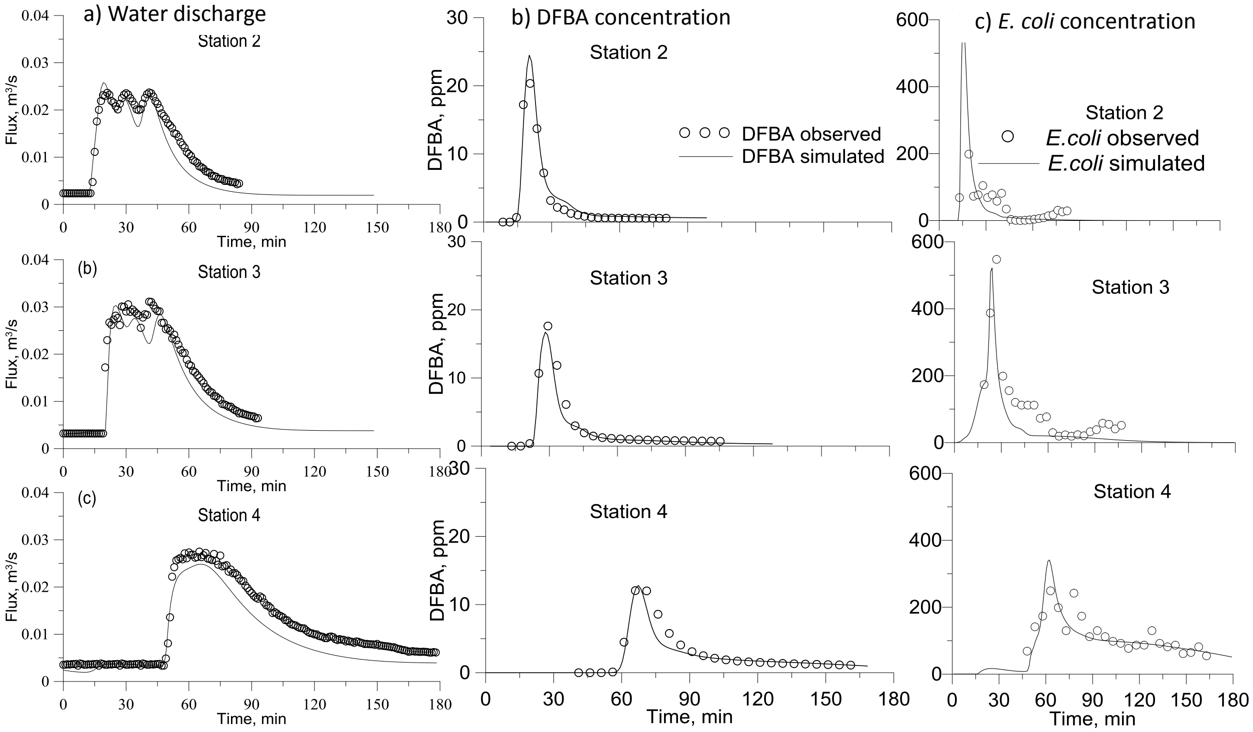

Figure 2 Observed and simulated a) water discharge, b) BTCs of DFBA tracer concentration and c) BTCs of *E. coli* concentration at three stations in the Beaver Dam Creek Tributary in 2009.

Folders MaSTiS-DFBA 2009 and MaSTiS-Ecoli 2009 include input and output data files for DFBA and *E. coli* simulations, respectively.

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