STWIR, a Microorganism Transport with Infiltration and Runoff add-on Module for the KINEROS2 Runoff and Erosion Model

Documentation and User Manual

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Abstract

Runoff from manured fields is often considered to be the source of microorganisms in the surface water used for irrigation, recreation, and household needs. Concerns of microbial safety of this water resulted in development of predictive models for estimating the concentrations and total numbers of pathogen and indicator organisms leaving manure fertilized fields in overland flow during runoff events. The KINEROS2 surface flow model (Woolhiser et al., 1990; Semmens et al., 2008; www.tucson.ars.ag.gov/kineros) was developed to simulate event based runoff from small agricultural and urban watersheds. The purpose of this technical bulletin is to describe the STWIR (Simulator of Transport With Infiltration and Runoff) microorganism routing add-on module for KINEROS2. Surface runoff transport of soil and manure-born microorganisms are computed based on advection-dispersion equations (module STWIR) coupled with the kinematic wave equation (module KINEROS2). The model and the necessary modifications of the KINEROS2 code are presented.

Disclaimer

Contents

Note on Units

The generic symbol MCU (microbial count units) 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, MCU may mean cells, CFU (colony forming units), PFU (plague forming units), cysts, genomes, etc.

Abbreviations

CFU – colony forming units (equivalent of cell number), FC – fecal coliforms, MCU – microbial count units

List of symbols

α_m the parameter controlling rate of microorganism release from manure, (hr^{-1});

a_L the dispersivity, (cm);

β_m the parameter controlling microorganism release from manure, (dimensionless);

μ_m the microorganism die-off rate in applied manure, (h^{-1});

μ_r the microorganism die-off rate in runoff water, (h^{-1});

μ_s the microorganism die-off rate in soil, (h^{-1});

μ_w the microorganism die-off rate in the mixing zone water, (h^{-1});

C_0 the initial content of microorganisms in applied manure, (MCU cm^{-3});

C_{ir} the microorganism concentration in irrigation water, (MCU cm^{-3});

C_r the microorganism concentration in runoff water, (MCU cm^{-3});

C_s the microorganism concentration in soil mixing zone, (MCU cm^{-3});

E_r the microorganism release efficiency, (dimensionless)

d the thickness of the topsoil layer that actively interacts with the overland flow, (cm);

h the depth of water ponding, (cm);

h_m the thickness of the applied manure, (cm);

I the infiltration rate, (cm h^{-1});

k the rate of microorganism exchange between the runoff water and the mixing zone in soil, (cm h^{-1});

k_a the attachment rate of microorganism at the solid phase, (h^{-1});

k_d the detachment rate of microorganism at the solid phase, (h^{-1});

k_f the fraction of infiltrated microorganisms which filtered out by the soil mixing zone, (dimensionless);

k_{str} the microorganism straining coefficient in soil,(dimensionless);

q the water discharge per unit width (cm^2 h^{-1});

R the irrigation rate, (cm h^{-1});

S_m the microorganism concentration in the manure applied to the soil surface (MCU cm^{-2});

S_s the microorganism concentration on the solid phase of soil mixing zone, (MCU g^{-1});

t time, (h);

x the distance along the slope, (cm);

ρ the topsoil bulk density, (g cm^{-3});

1. Introduction

Runoff from manured fields is often considered to be the source of microorganisms in the surface water used for irrigation, recreation, and household needs. Concerns for microbial safety of this water resulted in development of predictive models for estimating the concentrations and total numbers of pathogen and indicator organisms leaving manure fertilized fields in overland flow during runoff events. Such models of microorganism fate and transport have been developed and incorporated into watershed-scale water quality models including HSPF (Bicknell *et al.*, 2000), SWAT (Sadeghi and Arnold, 2002; Neitsch *et al.*, 2005), and other models developed specifically for pastureland watersheds (Tian *et al.*, 2002; Collins and Rutherford, 2004). The watershed scale approach received a lot of attention in modeling microbial water quality due to regulatory requirements such as the Total Maximum Daily Load, or TMDL program that was established to respond to the Clean Water Act of 1973 for nutrients and sediment as well as microbial water contaminants. The development of this new module of microorganism transport was motivated mostly by studies conducted at small scale (plot, field) within short time intervals (hours), where interactions of microorganism transported in runoff with microorganism resided in the soil pore solution and associated with the soil solid phase are important.

The purpose of this technical bulletin is to describe the STWIR (Simulator of Transport With Infiltration and Runoff) microorganism routing add-on module for KINEROS2. The KINEROS2 surface flow model (Woolhiser et al., 1990; Semmens et al., 2008; www.tucson.ars.ag.gov/ kineros) was developed to simulate runoff from small agricultural and urban watersheds.

Surface runoff transport of soil and manure-born microorganisms is computed based on advection-dispersion equations (module STWIR) coupled with the kinematic wave equations (module KINEROS2) and includes simulation of the following processes:

- microorganism release from surface applied manure;
- influx of microorganism from irrigation water;
- advective-dispersive transport of microorganism with runoff water;
- infiltration of microorganism into the soil;
- straining of microorganisms from the infiltrating water by plant litter and vegetation layer;
- exchange of microorganisms between runoff water and the mixing zone of soil at the surface;
- attachment and detachment of microorganism at the solid phase;
- microorganism die-off in manure, runoff water, soil mixing zone and soil solid phase.

The model complexity depends on application requirements and data availability. Any above listed process can be excluded from consideration by setting the corresponding parameters to zero. The model description and the necessary modifications of the KINEROS2 code are presented. The full KINEROS manual and supporting publications can be accessed at www.tucson.ars.ag.gov/kineros and will not be repeated here.

This report consists of:

1. Brief description of the mathematical models of the processes involved,
2. Description of the program structure and the data requirements for microorganism transport simulation,

3. Description of the modifications made in the KINEROS code,
4. Examples to help users to better understand the model inputs and generated output information.

2. Theory

2.1. Modeling overland water flow (KINEROS2)

The overland water flow component of the KINEROS2 model is described by the kinematic wave equation (Woolhiser et al., 1990),

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = R - I \qquad (1)$$

where *h* is the depth of ponding (m), *q* is the water discharge per unit width (m^2 s^{-1}), *R* is the precipitation rate (m s^{-1}), *I* is the infiltration rate (m s^{-1}), *t* is time (s), and *x* is the distance along the slope (m).

The depth-discharge relationship used is often expressed as

$$q = \alpha h^m \qquad (2)$$

where the parameter α is computed according to Manning (3) or Chezy (4) hydraulic resistance law as

$$\alpha = n^{-1} S^{1/2} \qquad \text{m=5/3} \qquad (3)$$

$$\alpha = C S^{1/2} \qquad \text{m=3/2} \qquad (4)$$

where *S* is the surface slope, (m m^{-1}), *n* is the Manning's roughness coefficient for overland flow, and *C* is the Chezy friction coefficient.

The Parlange et al. (1982) equation is used for calculating infiltration rate through the soil surface

$$I = K_s \left[1 + \frac{\sigma}{\exp\left(\sigma I^* / B\right) - 1} \right] \qquad (5)$$

where K_s is the saturated hydraulic conductivity (m s^{-1}), σ is the dimensionless parameter that represents the soil texture, I^* is the infiltrated depth (cm), $B = (G + h)(\theta_s - \theta_i)$, *G* is the net capillary drive (cm), θ_s and θ_i are the soil volumetric water contents at saturation and initial condition (cm^3 cm^{-3}), respectively.

2.2. Modeling overland transport and removal of microorganism (STWIR)

Two models of microorganism-soil interaction are considered in the STWIR add-on module. The first model assumes that microorganism exchange between the runoff water and soil solid phase occurs through the solution in the thin top soil layer (mixing zone). This model is designed for the studies conducted in runoff-boxes and at plot scales. The second model considers a direct interaction of microorganism suspended in the runoff water with the soil surface and is developed for field and watershed scales. This model ignores microorganism in the liquid phase of the mixing zone to eliminate high uncertainty of simulation introduced by spatial variability of water content in the top soil layer at large scales.

2.2.1. *Model of microorganism overland flow with exchange through the soil mixing zone*

The mass balance of the overland movement of microorganism for the first model has the form

$$\frac{\partial hC_r}{\partial t}+\frac{\partial qC_r}{\partial x}=\frac{\partial}{\partial x}\left(a_L q\frac{\partial C_r}{\partial x}\right)+kh(C_s-C_r)-(1-k_{str})IC_r+RC_{ir}+RC_m-\mu_r hC_r \quad (6)$$

where C_r and C_s are the microorganism concentration in the runoff water and in the soil mixing zone (MCU cm^{-3}), respectively, a_L is the dispersivity (m), k is the rate of mass transfer (s^{-1}), k_{str} is the straining coefficient, C_{ir} is the microorganism concentration in irrigation water (MCU cm^{-3}), C_m is the concentration of microorganism released from manure (MCU cm^{-3}), and μ_r is the microorganism die-off rate in the runoff water (s^{-1}).

The first and the second terms in the left-hand side of (6) describe the change of microorganism concentration in overland flow, while the second term accounts for the microorganism advection with the velocity calculated by (2). In the right-hand side, the first term describes the microorganism dispersion assuming its linear dependence on the advective flux; the second term accounts for the exchange of microorganisms between runoff water and the mixing zone of soil at the surface; the third term simulates straining of microorganisms from the infiltrating water by plant litter and the vegetation layer (assumed to be proportional to the infiltration rate *I*, the coefficient k_{str} $0 \le k_{str} \le 1$ is a lumped parameter that accounts for the rate of straining, k_{str}=0 no straining occurs); the fourth and fifth terms describe influx of microorganism, if present, from rain or irrigation water; and the last term accounts for the microorganism die-off in runoff water.

The concentration of released microorganism C_m is calculated according to Bradford and Schijven (2002) as

$$\begin{aligned} C_{man}(t) &= \frac{dM_{man}}{Rdt} = \frac{M_0\alpha_m}{R}(1+\alpha_m\beta_m t)^{-(1+1/\beta_m)} \\ C_m(t) &= m_i E_r C_{man}(t) \end{aligned} \qquad (7)$$

where M_{man} is the cumulative manure mass released into the aqueous phase (g), α_{m} (h^{-1}) and β_m are dimensionless fitting parameters defining the shape of the release curve, and M_0 is the initial mass of manure (g), C_{man} is the aqueous manure concentration (g cm^{-3}), m_i is content of microorganism in the applied manure (MCU g^{-1}), E_r is microorganism release efficiency.

The microorganism die-off in the surface applied manure is described as

$$\frac{\partial m_i}{\partial t} = -\mu_m m_i \qquad (8)$$

where μ_m is the microorganism die-off rate in applied manure, (s^{-1});

The mass balance equations of microorganism transport in the mixing zone of the topsoil are:

$$d\frac{\partial(\theta C_s)}{\partial t}+\rho d\frac{\partial S_s}{\partial t}=-kh(C_s-C_r)+(1-k_{str})IC_r-d\mu_w C_s-(1-k_{str})IC_s \qquad (9)$$

$$\rho\frac{\partial S_s}{\partial t}=\theta k_a C_s-k_d\rho S_s-\rho\mu_s S_s \qquad (10)$$

where S_s is the microorganism concentration on the solid phase of soil mixing zone (MCU g^{-1}), k_a and k_d are the attachment and detachment rates of microorganism at the solid phase (s^{-1}), respectively, ρ is the topsoil bulk density (g cm^{-3}), and d is the thickness of the mixing zone, i.e. topsoil layer that actively interacts with the overland flow (m), μ_w and μ_s are microorganism die-off in the soil mixing zone and the solid phase, respectively, (s^{-1}).

The first and second terms in the left-hand side of (9) describe change of microorganism concentration in the liquid and solid phases of the mixing zone, respectively; the first and second term in the right-hand side account for exchange of microorganisms with the overland flow and their influx with the infiltrated water, respectively. The third term accounts for microorganism die-off in the liquid phase of mixing zone. Equation (10) describes reversible attachment and detachment of microorganism (the first and second term in the right-hand side, respectively) to the solid phase in the mixing zone. The third term accounts for microorganism die-off in the solid phase of mixing zone.

2.2.2. *Model of microorganism overland flow with direct interaction between microorganism suspended in the runoff water and the soil surface*

The mass balance of the overland movement of microorganism for the second model has the form:

$$\frac{\partial hC_r}{\partial t} + \frac{\partial qC_r}{\partial x} = \frac{\partial}{\partial x}\left(a_L q \frac{\partial C_r}{\partial x}\right) - d(\theta k_a C_r - k_d \rho S_s) - (1 - k_{str})IC_r + RC_{ir} + RC_m - \mu_r hC_r \quad (11)$$

where d is the thickness of the soil surface layer that actively interacts with the overland flow (cm).

The left side of equation (11) is similar to the left side of Eq. (6). In the right-hand side, the second term has been changed and describes the exchange of microorganisms between runoff water and the soil surface layer.

The mass conservation equation of microorganism in the soil surface layer is:

$$d\rho \frac{\partial S_s}{\partial t} = d(\theta k_a C_r - k_d \rho S_s) + k_f (1 - k_{str})IC_r - d\rho\mu_s S_s \quad (12)$$

where k_f is the fraction of microorganisms which enter the soil mixing zone with the infiltrated water and are filtered out within this zone by the soil solid phase.

The left-hand side of equation (12) describes the change of microorganism concentration in the solid phase of the soil surface layer; the first term in the right-hand side describes reversible attachment and detachment of microorganism to the solid phase, the second term accounts for microorganism filtered out of infiltrated water by soil solid phase, while the third term describes microorganism die-off in the soil solid phase.

The second model uses Eq. (7) and Eq.(8) to simulate microorganism release from the surface applied manure.

2.2.3. *Boundary conditions and numerical solution*

The set of equations (1) to (12) is solved numerically using the implicit finite difference scheme. Initial and boundary conditions were set as described below. The KINEROS2 numerical code solves the infiltration and runoff flow equations (1-5) with the boundary conditions of zero water ponding depth h at x=0, and the initial condition of h=0 for x>0 were used. The front limitation algorithm (Haefner et al., 1997) was applied to solve the microorganism transport equations (6) - (12). The Dirichlet boundary condition of zero concentration and the Neumann boundary condition of zero concentration gradient were set at the inlet and outlet boundaries, respectively, and the constant initial concentration C_r=0 at x>0 was assumed for Eq.(6) and Eq.(11).

3. STWIR program documentation

3.1. Program structure description

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

Table 1. STWIR subroutines

Subroutines	Functions
STWIR	Solves the microorganism transport equations (6) – (12). Calls from FCTRANSPORT.
GRID	Creates a numerical grid for microorganism transport and converts input parameters into format used in STWIR module. Calls from PLANE.
FCTRANSPORT	Sends results of water flow simulation to STWIR subroutine. Calls from PLANE

An additional input file is required to run STWIR module. Detailed file description follows.

3.2. Modification of the KINEROS2 source code

The code modifications are marked as "!AG" throughout the KINEROS2 code.

<u>K2shell.f90</u>

1. Added Input/output microorganism files

    character(len=20) :: Chemfile, resfile

2. Read Input and Output files for microorganism transport

    read(4, 10) Chemfile

    read(4, 10) resfile

3. Update kin.fil

```
write(4, 10) Chemfile

write(4, 10) resfile
```

4. Open Input and Output files for microorganism transport

```
open(10, file = Chemfile, status = 'old', iostat = file_error)

if(file_error .ne. 0) call errxit('K2shell',"Can't open "//Chemfile)

open(11, file = resfile)
```

<u>Kineros2.for</u>

1. Added Common blocks for microorganism subroutine

```
Character*80 comments

Common /ParamFC/ ind,fPar(20)

Common /PlanVar/ nk
```

2. Input title for microorganism variables

```
read(10,*) comments
```

3. Read microorganism parameters for each segment ID and Print title for output file:

```
      read(10,*) ID,ind,nk,(fPar(i),i=1,16)

      write(11,'(/"Segment",i3/," Time    Cum Runoff  Cum Runoff FC runoff

   *  FC total")') ID

      write(11,'(" (min)     (m^3)      (mm)      MCU         MCU")')
```

<u>Plane.for</u>

1. Increased array dimensions:

```
common /plane1/ dt, dx, j, jp1, qlav, alpha(200), p(200), h1(200),
```

```
&          h2(200), q1(200), q2(200), h2c, ams, wpc, c1, c2,
&           bw, qb, omega
real,dimension(100,2) :: qup
real,dimension(200,2) :: ql
```

2. Added common block for number of spatial nodes and array to store FC concentrations time series at the end of each segment:

```
Common /PlanVar/ nk
Real Cout(20,5000)
```

3. Total microorganism amount in runoff at the end of segment:

```
Tbact = 0.0
```

4. Modified nk for fine resolution in microorganism transport subroutine:

```
nk=min(nk,200)
C     nk = max1 ((15. * xleng / clen), 5.)
C     if (nk .gt. 15) nk = 15
```

5. Generated grid and assigned parameters for microorganism STWIR:

```
call Grid(dx,nk)
```

6. Read Inflow (qub2) and concentration (Co) from upstream area [cc m/s]:

```
if (up) then
        call get (upq, i, qub2)
        Co=Cout(idup,i)
      else
        qub2 = 0.0
        Co = 0.0
```

```
end if
```

7. Call “FCtransport” Microorganism Transport subroutine:

```
call FCtransport(time,dte,rf,fav,Co,Cn)
```

8. Accumulate microorganism amount in runoff at the end of the segment:

```
Tbact = Tbact + Cn * qout2 * dt
```

9. Print out results of microorganism transport simulation

```
Cout(id,i) = Cn
RunoffVol = qbal(10) * width
RunoffDepth = 1000.0 * RunoffVol/coarea
write(11,'(F6.1,2F12.5,3G14.6)') time/60,RunoffVol,RunoffDepth,
* Co/1.e+6,Cn/1.e+6,Tbact
```

<u>Infilt.for</u>

1. Added Common block to pass porosity (fPar(20)) to Subroutine FCtransport

```
Common /ParamFC/ ind,fPar(20)
```

2. Topsoil porosity

```
fPar(20) = por1(i)
```

The source code was compiled with Compaq Visual Fortan v. 60, DIGITAL Visual Fortran Professional Edition 6.0.0 and Fortran Power station 4.0 compilers

3.3. Input data

The input data for STWIR are given in two input files. These are the KINEROS *kin.fil* file and the input file that contains the microorganism transport parameters. The name of the second file is user specified in *kin.fil* (line 3). All input files must be placed into one directory.

The STWIR information that needs to be supplied in *kin.fil* file is shown in Table 2. Lines 1, 2 and from 5 through 13 is the input of the original KINEROS. The additional information needed for SRWIR is added on lines 3 and 4. These are the names of the input and output files used in STWIR.

Table 2. *KINEROS2 Project input file kin.fil. The STWIR inputs are shown in bold.*

Line	Data Type	Description
1	Character	KINEROS parameter file (see *Input.pdf*)
2	Character	Rainfall data file (see *Input.pdf*)
3	**Character**	**Microorganism transport parameters input file**
4	**Character**	**Microorganism transport output file**
5	Character	KINEROS output file
6	Character	Project title
7	Numerical	Length of Run, minutes
8	Numerical	Time Step, minutes
9	Character	Use Courant criteria? (y or n)
10	Character	Simulate Sediment Transport? (y or n)
11	Character	Multiplier file (if any) (y or n)
12	Character	Tabular Summary? (y or n)
13	Character	API Initializing? (y or n)

A new input file must be created to specify parameters of the STWIR module. The input file includes NELE+1 lines, where NELE is the number of simulation elements defined in the KINEROS2 input file. The first input line lists names of the variables used for the microorganism transport simulation. The following lines contain the values of the model parameters described in Table 3. Their order corresponds to the sequence of elements listed in the KINEROS parameter file.

Table 3. *STWIR module data file*

Variable	Description	Units
ID	Element identification number corresponding to KINEROS ID	-
IND	Microorganism transport Model number: IND=1 - no microorganism transport with runoff, IND=2 - Model 1, IND=3 - Model 2	-
Nk	Modified number of nodes for fine resolution in microorganism transport subroutine (200 maximum)	-
Lam	Dispersivity a_L	m
Kf	Model 1 - microorganism exchange rate between runoff and soil water (k) Model 2 - fraction of infiltrated microorganism which filtered out by the soil mixing zone ($k_f=0\text{-}1$)	1/h -
Ka	Attachment rate of microorganism at the solid phase (k_a)	1/h
Kd	Detachment rate of microorganism at the solid phase (k_d)	1/h
Kstr	Distribution coefficient for microorganism infiltration ($k_{str}=0\text{-}1$)	
Aman	The parameter defining the rate of the microorganism release from manure (α_m). If Aman=0 an empirical relationship $\alpha_m = 0.036 + 0.860\,R$ is used.	1/h
Bman	The fitting parameter defining the shape of the microorganism manure-release curve (β_m)	-
Er	The microorganism release efficiency (E_r)	-
Cm	The initial microorganism content in the applied manure (C_0).	MCU/cm^2
So	The initial microorganism content in the soil (S_s).	MCU/g
D	Depth of exchange zone (d)	m
Cir	Microorganism concentration in irrigation water (C_{ir})	MCU/ml
Mum	The microorganism die-off rate in applied manure (μ_m)	1/h
Mur	The microorganism die-off rate in runoff water (μ_r)	1/h
Mus	The microorganism die-off rate in soil (μ_s)	1/h
Muw	The microorganism die-off rate in the mixing zone water (μ_w)	1/h

* Units in the input file differ from units used in the subroutine STWIR

3.4. STWIR output file

The STWIR module creates a new output file. The file is named as listed in line 4 of the KINEROS2 project input file *kin.fil.* The output file contains the results of microorganism transport simulations separately for each plane (overland flow) model element in the format listed in Table 4.

Table 4. *Format of the output data generated by the STWIR module*

Line	**Content**
1	Blank
2	Plane element number
3	List of output variables
4	Units for output variables
5 … n	Time, Cum Runoff, Cum Runoff, Co, Cn, FC total (see Table 5 for detailed description).

Table 5. *List of the output variables*

Time (min)	Time from the beginning of simulation
Cum Runoff (m^3)	Total runoff volume from the plane model element.
Cum Runoff (mm)	Total runoff depth from the plane model element based on the contributing area
Co (MCU/ml)	Microorganism concentration in the inflow water at the first node of the plane model element
Cn (MCU/ml)	Microorganism concentration in the outflow water at the last node of the plane model element
FC total (MCU)	Total amount of microorganism released from the plane model element

4. Example problems

Two example problems demonstrating the STWIR module application are presented in this section. Example 1 demonstrates the application of the model of microorganism overland flow with exchange through the soil mixing zone (Model 1) for the scale of the irrigation plot. Example 2 demonstrates application of the model based on the direct interaction of microorganism suspended in the runoff water with the soil surface (Model 2) at a field scale.

4.1. Example 1 – Plot scale test

In this example the model reproduces the results of the overland flow experiments with the manure-borne fecal coliforms (FC) carried out in October 2003 on a lysimeter located at the USDA-ARS facility in Beltsville, Maryland (Guber et. al, 2009). The slope of the lysimeter surface was 20% (Fig.1). The lysimeter had clay loam soil texture and was planted with a mixture of blue fescue (*Festuca ovina 'Glauca'*) and white clover (*Trifolium repens*). Plots 2 m wide and 6 m long were established to study FC transport with runoff through a vegetation filter strip. The bovine manure slurry was manually applied on the top of the plots in a 30-cm wide strip at the rate of 11.7 L m^{-2}. Rainfall simulations were started immediately after manure application. Rainfall rates were 54 and 59 mm h^{-1} at top 30-cm strip and at the area below, respectively. Rainfall was simulated for one hour after the initiation of runoff. Runoff samples were collected in troughs, located at the bottom of the plots for 2 minutes, at 5-minute intervals. Runoff volume and fecal coliform (FC) concentrations were measured for each runoff sample. The colony forming units (CFU) were used to express the FC contents, i.e. MCU were CFU in this case.

The hydraulic component of the KINEROS2 model (Eqs. 1-4) was calibrated for the observed cumulative runoff depth. The Manning's roughness coefficient (n), parameters K_s, σ

and *G* of the Parlange equation (5) were estimated during the calibration using PEST software (Doherty, 2005). The model after calibration performed satisfactorily as shown in Fig. 2a. The value of the root mean square errors (RMSE) for the cumulative runoff depth was 3.7 cm. Pearson correlation coefficient between measured and simulated data was 0.999.

The transport component of STWIR was then calibrated using measured FC concentrations in the runoff water. The thickness of the soil mixing zone was set to 1 cm. The STWIR parameters a_L, k, k_a, k_d, k_s , k_f, and β_m (Eqs. 6-10) were fitted to the measured FC concentrations. We assumed that microorganism die-off within 2-hr experiment did not affect FC concentrations in runoff. Therefore die-off parameters μ_r, μ_m, μ_w, and μ_s were set to be equal to zero. The calibration resulted in the satisfactory performance of the STWIR model (Fig. 2b). Relatively small RMSE (5.36 10^2 CFU ml^{-1}) and a high correlation coefficient (r = 0.630 at P = 0.02) indicated the ability of the model to simulate FC transport with overland flow. Calibrated values of the KINEROS2 and STWIR model are presented in Table 6.

Figure 1. Experimental setup for plot-scale overland flow experiments located at USDA-ARS facility in Beltsville, Maryland.

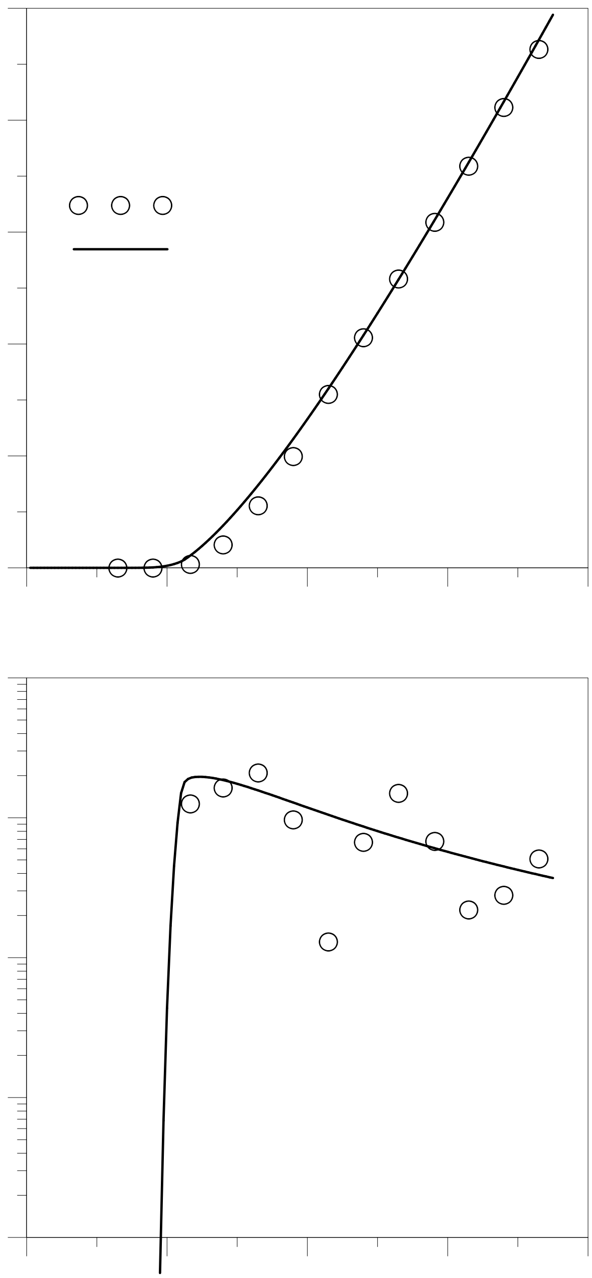
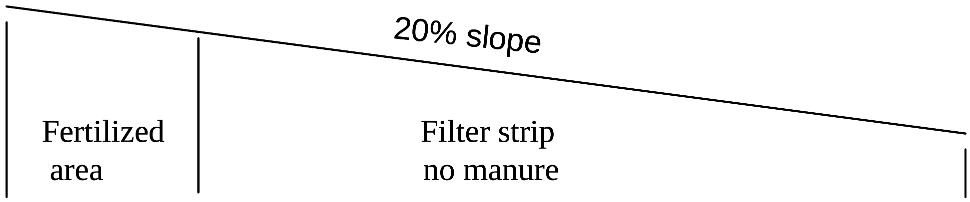


Figure 2. Measured and simulated cumulative runoff (a), and FC concentrations in runoff water (b) obtained in the Plot-scale test of the KINEROS2 and STWIR model.

Table 6. Input parameters for Example 1



Parameter	Plane 1	Plane 2
ID	1	2
UPSTREAM	-	1
LEN [m]	0.30	5.7
WID [m]	2.0	2.0
SL	0.20	0.20
n	0.41	0.41
CV	0.1	0.1
THICK	1000.0	1000.0
SAT	0.42	0.42
PR	2	2
RELIEF	0.0	0.0
SPACING	0.3	0.3
K_s [cm/h]	20.0	30.0
G [cm]	96.3	96.3
σ	1.0	1.0
Por [cm^3/cm^3]	0.419	0.419
ROCK	0.0	0.0
nk	180	180
Lam [m]	0.5	0.5
Kf	0.027	0.027
Ka [1/h]	11.2	11.2
Kd [1/h]	0.0	0.0
Kstr	1.0	1.0
Aman [1/h]	20.0	0.0
Bman	1.0	0.0
Cm [CFU/cm^2]	$2x10^8$	0.0
Er [-]	1.0	0.0
So [CFU/g]	0.0	0.0
Crain [CFU/ml]	0.0	0.0
d [m]	0.01	0.01
Mum [1/h]	0.0	0.0
Mur [1/h]	0.0	0.0
Mus [1/h]	0.0	0.0
Muw [1/h]	0.0	0.0

INPUT DATA

The input data for KINEROS2 and STWIR are given in 5 separate files of subdirectory: ..\STWIR\ Plot_scale_test. File format used in STWIR module (*Plot-FC.par*) is described in Table 2 and 3 of this manual. For the KINEROS2 input format (*kin.fil*, *milt.fil*, *Plot-Soil.par* and *Irrigation.pre*) please refer to Woolhiser et al. (1990). The input files for this example must be placed into the same subdirectory and arranged as follows:

File *kin.fil*

Plot-Soil.par
Irrigation.pre
Plot-FC.par
Plot-Runoff.out
Plot-FC.out
Test 1: FC transport with runoff from a Clay loam vegetated plot
75
0.5
y
y
m
n
n

File *mult.fil*

1.0
1.0
1.0
1.0
1.0
1.0
1.0

File *Plot-Soil.par*

BEGIN GLOBAL

CLEN = 6.0, UNITS = METRIC

DIAMS = .005, .05, .25 ! mm

DENSITY = 2.65, 2.60, 2.60 ! g/cc

TEMP = 33 ! deg C

```
 Nele = 2

END GLOBAL
!-----------------------------------------------------
BEGIN PLANE ! Manure fertilized area

 ID = 1,  LEN = 0.3,  WID = 2,  SL = .2,  MANNING = .41

 X=0.0, Y=0.15

 CV = 0.1,    THICK = 1000., SAT = .42,  PR = 2

 RELIEF = 0.0,  SPACING = .3

 KS       G       DIST    POR      ROCK
 20.0     96.3    0.1    .419     0      ! upper layer

 FRACT = 0.2, 0.6, 0.2    SPLASH = 50,  COH = 0.5

 Plot = H
END PLANE
!-----------------------------------------------------
BEGIN PLANE ! Filter strip

 ID = 2,  UPSTREAM = 1,  LEN = 5.7,  WID = 2,  SL = .2,  MANNING = .41

 X=0.0, Y=3.15

 CV = 0.1,    THICK = 1000., SAT = .42,  PR = 2

 RELIEF = 0.0,  SPACING = .3

 KS       G       DIST    POR      ROCK
30.0     96.3    0.1    .419     0      ! upper layer

 FRACT = 0.2, 0.6, 0.2    SPLASH = 50,  COH = 0.5

 Plot = H
END PLANE
```

File ***Irrigation.pre***

```
BEGIN RG001

  N = 3
```

```
   TIME        DEPTH
!  (min)       (mm)

    0.0         0.00
   75.0   68.1
   79.0   68.1
X=0.0, Y=0.15
END
BEGIN RG002

  N = 3

   TIME        DEPTH
!  (min)       (mm)

    0.0         0.00
   75.0   74.6
   79.0   74.6
X=0.0, Y=3.15
END
```

File *Plot-FC.par*

ID	IND	nk	lam	Kf	Ka	Kd	Kstr	Aman	Bman	Cm	Er	So	Crain	d	Mum	Mur	Mus	Muw
1	2	6	0.50	0.027	11.2	0.0	1.0	20.0	1.0	2.E+08	1.0	0.0	0.0	0.01	0.0	0.0	0.0	0.0
2	2	115	0.50	0.027	11.2	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0.0	0.0	0.0	0.0

OUTPUT DATA

Output data will be in the files *Plot-FC.txt* and *Plot-Runoff.txt* placed into subdirectory:..\STWIR\ Plot_scale_test. The file names are specified in the input file *kin.fil.* Format of the file produced by STWIR module (*Plot-FC.txt*) is described in Table 4 and 5 of this manual. For format of the KINEROS2 output file (*Plot-Runoff.txt*) please refer to Woolhiser et al. (1990).

4.2. Example 2 – Field scale test

This example reproduces the results of the study of FC transport in the overland flow after manure application conducted at the OPE3 USDA-ARS research site (Beltsville, Maryland) in May 2004 (Guber et. al, 2011). The soil in the study area is classified as a coarse loamy, siliceous, mesic Typic Hapluddults. The soil profile consists of coarse loamy sand in the top soil (0-30 cm) with organic matter content of 1-2%, underlain with sandy loam (30-80 cm), coarse sand (80-150 cm), and gravelly sand in the lowest horizon (150-250 cm).

An H-flume, 0.457-m deep, was installed at the lowest point of the field to record runoff hydrographs (Fig. 3). The flume was equipped with a SIGMA 900 MAX refrigerated sampler (Hach Co, Loveland, CO, USA) to collect runoff water for the microorganism analysis. Precipitation was measured at a distance of approximately 100 m from the experimental field with a TE525 tipping-bucket rain gauge (Texas Electronics, Dallas, Texas).

Manure collected from the dairy and beef herd production center in Beltsville, MD was applied at a 59.3 ton/ha application rate on the 3.55 hectare experimental field on May 2. During the application the Eastern edge of the field (approximately 10 m from the flume) did not receive manure. Manure and soil samples were taken from the top 5 cm soil layer randomly across the field to measure FC content. FC content in all soil samples was below the detection limit. FC content in the applied manure was $4.25 \cdot 10^6$ CFU/g of wet manure, which was equivalent of $2.51 \cdot 10^6$ CFU/cm^2 of applied area.

A runoff event was observed during and after intensive rainfall on May 10. Total precipitation of 21.1 mm resulted in total runoff of 1.41 mm. Ten runoff samples were collected during the event to measure FC concentrations in the runoff water.

The Arc/Info GIS hydrologic modeling tool Watershed (ESRI Hydrology Modelling Tools v.2) was applied to a raster grid of the surface elevation to delineate the upslope area contributing flow to the flume (Fig. 3). The delineated area of 1.60 ha was represented in the KINEROS2 model as a 84.1x190.0 m rectangular overland flow plane with a slope of 2.7% toward the flume to simulate FC transport with overland flow. The rectangle was subdivided into two planes of 180-m and 10-m long, respectively. Both planes had the same soil properties. This allowed accounting for the area which did not receive manure during the application.

The hydraulic component of the KINEROS2 model (Eqs. 1-4) was calibrated for the observed runoff. The Chezy friction coefficient (C), and parameters K_s, σ and G of the Parlange equation (5) were estimated during the calibration using PEST software (Doherty, 2005). After calibration the model performed satisfactorily (Fig. 4a). Root mean square error (RMSE) for the cumulative runoff was 0.042 cm. The Pearson correlation coefficient between measured and simulated data was 0.998.

The transport component of STWIR was then calibrated using measured FC concentrations in the runoff water. The thickness of the soil mixing zone was set to 1 cm. The STWIR parameters a_L, k_a, k_d, k_s , k_f, and β_m (Eqs. 11-12) were fitted to the measured FC concentrations. The die-off parameters μ_{r}, μ_{m}, μ_{w}, and μ_{s} were set to be equal to zero similar to the runoff plot-scale test. This helped to avoid the effect of overparameterization. The calibration resulted in the satisfactory performance of the STWIR model (Fig. 4b). A relatively small RMSE ($8.0 \cdot 10^2$ CFU ml^{-1}) was computed with a relatively high value of the Nash-Sutcliffe efficiency (0.74) and a high correlation coefficient (0.87) which indicated ability of the model to simulate FC transport with overland flow. Calibrated values of the KINEROS2 and STWIR model are presented in Table 7.

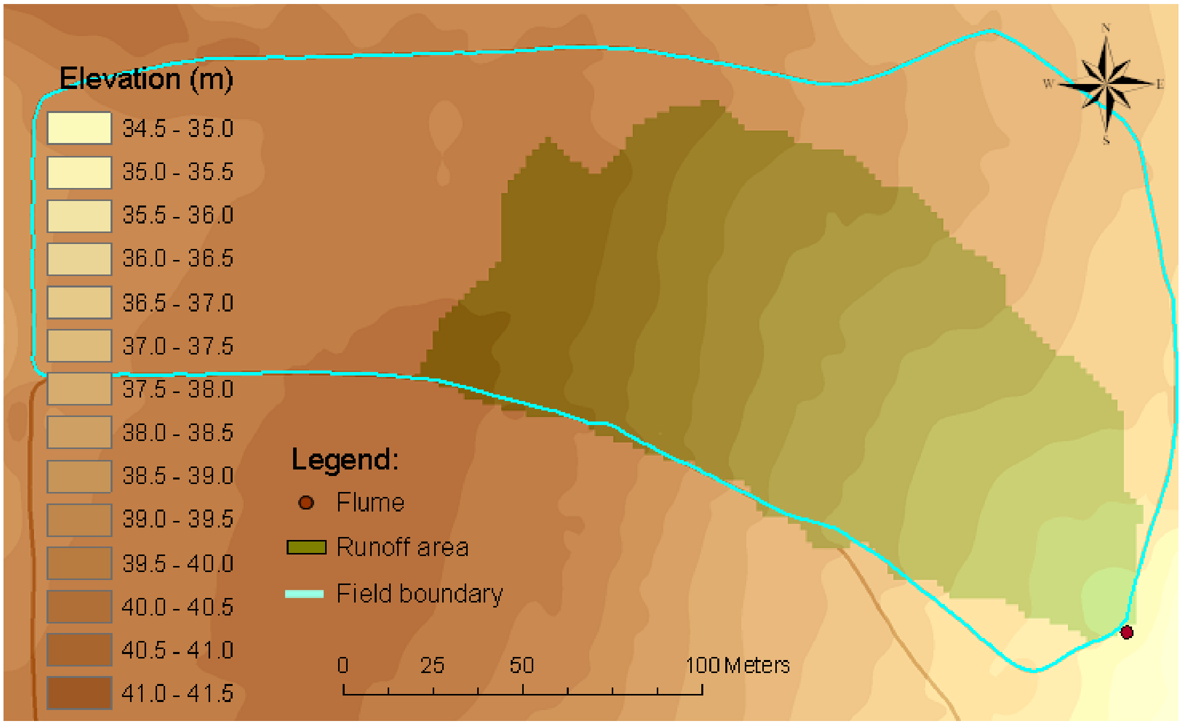


Figure 3. Digital elevation map of the study area.

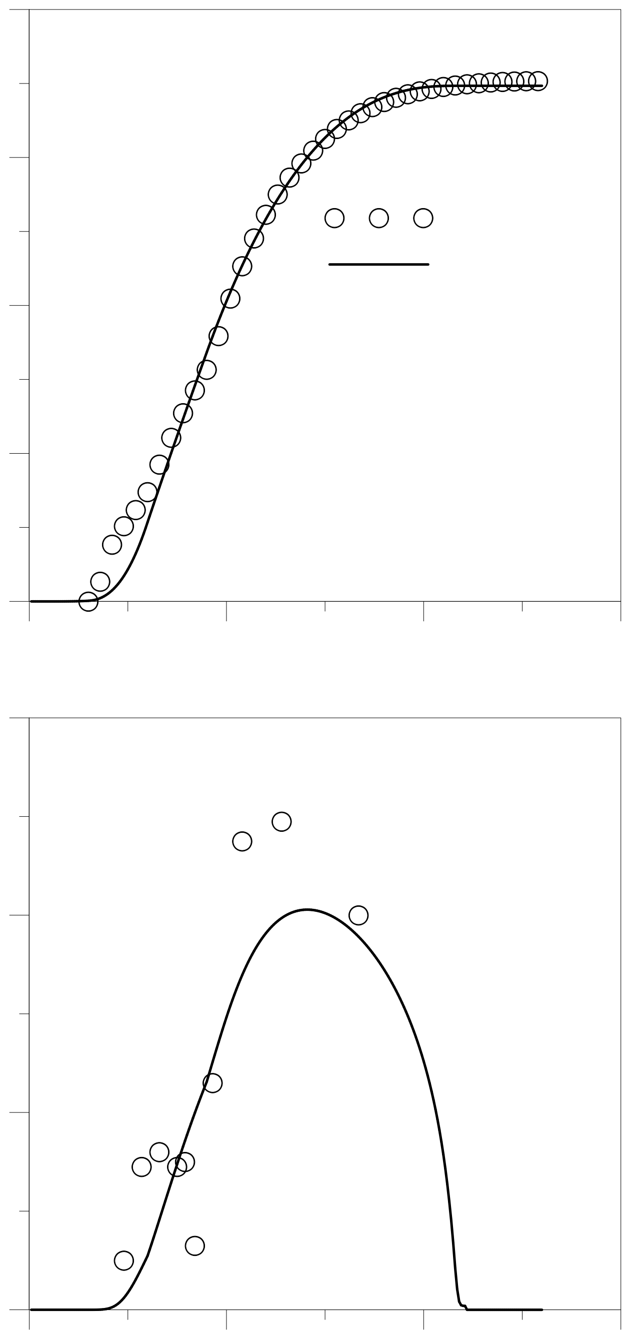
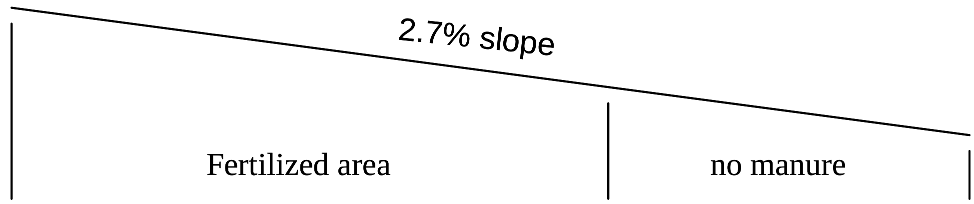


Figure 4. Measured and simulated cumulative runoff (a), and FC concentrations in runoff water (b) obtained in the Field- scale test of the KINEROS2 and STWIR model.

Table 7. Input parameters for Example 2.



Parameter	Plane 1	Plane 2
ID	1	2
UPSTREAM	-	1
LEN [m]	180	10
WID [m]	84.1	84.1
SL	0.027	0.027
C	0.259	0.259
CV	0.1	0.1
THICK	1000.0	1000.0
SAT	0.47	0.47
PR	2	2
RELIEF	0.5	0.5
SPACING	0.3	0.3
K_s [cm/h]	4.834	4.834
G [cm]	10.0	10.0
σ	1.0	1.0
Por [cm^3/cm^3]	0.54	0.54
ROCK	0.0	0.0
nk	180	11
Lam [m]	3.53	3.53
Kf	0.1	0.1
Ka [1/h]	1.135	1.135
Kd [1/h]	0.005	0.005
Kstr	1.0	1.0
Aman [1/h]	0	0
Bman	0.15	0.15
Cm [CFU/cm^2]	$2.51x10^6$	0.0
Er [-]	1.0	0.0
So [CFU/g]	0.0	0.0
Crain [CFU/ml]	0.0	0.0
d [m]	0.01	0.01
Mum [1/h]	0.0	0.0
Mur [1/h]	0.0	0.0
Mus [1/h]	0.0	0.0
Muw [1/h]	0.0	0.0

INPUT DATA

The input data for KINEROS2 and STWIR are given in 5 separate files of subdirectory: ..\STWIR\ Field_scale_test. File format used in STWIR module (*Field-FC*) is described in Table 2 and 3 of this manual. For the KINEROS2 input format (*Field-Soil.par*, *mult.fil* and *Rain051004.pre*) please refer to Woolhiser et al. (1990). The input files for this example must be placed into the same subdirectory and arranged as follows:

File *kin.fil*

```
Field-Soil.par
Rain051004.pre
Field-FC.par
Field-FC.txt
Field-Runoff.txt
Field scale test of FC transport at OPE3 field for the event observed in May 10, 2004.
260.0
 1.0
y
n
m
n
n
```

File *mult.fil*

```
1.0
1.0
1.0
1.0
1.0
1.0
1.0
```

File *FieldA-Soil.par*

```
BEGIN GLOBAL

  CLEN =190,  UNITS = METRIC

  DIAMS = .005, .05, .25 ! mm
```

```
 DENSITY = 2.65, 2.60, 2.60 ! g/cc

 TEMP = 33 ! deg C

 Nele = 2

END GLOBAL
!-----------------------------------------------------
BEGIN PLANE

 ID = 1,  LEN = 180,  WID = 84.1,  SL = .027,  Chezy=0.259

 CV = 0.1,    THICK = 1000., SAT = .47,  PR = 2

 RELIEF = 0.5,  SPACING = .3

 KS      G      DIST    POR      ROCK
5.9     10.0     1.0        0.54         0      ! upper layer

 FRACT = 0.2, 0.6, 0.2    SPLASH = 50,  COH = 0.5

 Plot = H

END PLANE
!-----------------------------------------------------
BEGIN PLANE

 ID = 2,  UPSTREAM = 1, LEN = 10,  WID = 84.1,  SL = .027,  Chezy=0.259

 CV = 0.1,    THICK = 1000., SAT = .47,  PR = 2

 RELIEF = 0.5,  SPACING = .3

 KS      G      DIST    POR      ROCK
5.9     10.0       1.0    0.54          0      ! upper layer

 FRACT = 0.2, 0.6, 0.2    SPLASH = 50,  COH = 0.5

 Plot = H

END PLANE
```

File *Rain051004.pre*

BEGIN RG001

N = 5

TIME	DEPTH
! (min)	(mm)
0.0 0	
30.0	4.826
60.0	18.542
90.0	21.082
260.0	21.082

END

File *FieldA-FC.par*

ID	IND	nk	Lam	Kf	Ka	Kd	Kstr	Aman	Bman	Cm	Er	So	Crain	d	Mum	Mur	Mus	Muw
1	3	180	3.53	0.1	1.135	0.005	1	0.0	0.15	2.51E+06	1.0	0.0	0.0	0.01	0.0	0.0	0.0	0.0
2	3	11	3.53	0.1	1.135	0.005	1	0.0	0.15	0.0	0.0	0.0	0.0	0.01	0.0	0.0	0.0	0.0

OUTPUT DATA

The output data are in the subdirectory:..\STWIR\ Field_scale_test in the output files specified in the input file *kin.fil* as: *Field-FC.txt* and *Field-Runoff.txt.* Format of the file produced by STWIR module (*Field-FC.txt*) is described in Table 4 and 5 of this manual. For format of the KINEROS2 output file (*Field-Runoff.txt*) please refer to Woolhiser et al. (1990).

5. References

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