

MODELING RUNOFF POLLUTANT DYNAMICS THROUGH VEGETATIVE FILTER
STRIPS: A FLEXIBLE NUMERICAL APPROACH

By

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A la memoria de mi abuelito Alfredo Ovilla Gutiérrez, a quien recuerdo con mucho amor y respeto. (To the memory of my grandfather Alfredo Ovilla Gutierrez⁺, who I remember with much love and respect)

A mi esposa, Paola, por ser mi amor platónico y el ala que necesitaba para levantar el vuelo de mi vida...Tuyo soy. (To my wife, Paola, to be my love and the wing I needed to take the flight of my life...I am only yours.)

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LIST OF ABBREVIATIONS

ADR	Advection-Dispersion-Reaction Equation
CFA	Carbonate Flour Apatite
FEM	Finite Element Method
RSM	Regional Simulation Model
SFWMD	South Florida Water Management District
TaRSE	Transport and Reaction Simulation Engine
TR-FEM	Fully coupled Transport-Reaction model using Finite Elements Method.
VFS	Vegetative Filter Strips
VFSMOD-W	Vegetative Filter Strip Hydrology and Sediment Transport Modeling System
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
K_{CFA}	Dissolution rate of apatite from soil
SSA_{CFA}	Specific Surface Area of Carbonate Flour Apatite

LIST OF SYMBOLS

Γ	Sink/source term for the Advection-Dispersion-Reaction Equation
C	Pollutant Concentration, mg/l
C_p	Concentration of pollutant in surface runoff, mg/l
S_p	Concentration of pollutant in porewater, mg/l
C_{SW}^P	Surface water concentration of soluble reactive phosphorus, mg/l
C_{PW}^P	Soil porewater concentration of soluble reactive phosphorus, mg/l
S^P	Soil absorbed phosphorus
S^o	Phosphorus concentration in organic soil
C_s^P	Phosphorus as plankton biomass
C^{mp}	Phosphorus as macrophyte biomass
C_w	Bromide concentration in runoff, mg/l
C_e	Bromide concentration in porewater, mg/l
d_e	Exchange layer depth, m
D_L	Hydrodynamic dispersivity, m ² /s.
D_m	Molecular dispersion, m ² /s
α_L	Longitudinal dispersion, m
v	Flow velocity, m/s
t	Time, s
t_o	Initial time, s
x	Distance on plane x following the flow direction, m.
k_1	First order reaction coefficient, s ⁻¹
k_u, k_{st}	Uptake coefficient, s ⁻¹
k_r, k_{rs}	Release coefficient, s ⁻¹
Z_d	Water depth, m

p	Precipitation, m/s
f	Infiltration rate, m/s
q	Flow discharge, m ² /s
Q	Flow, m ³ /s
k _a	Apatite rate constant, moles m ⁻² s ⁻¹
ρ _b	Soil bulk density, g cm ⁻³
η	Porosity, cm ³ cm ⁻³

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Methods to estimate surface runoff pollutant removal using vegetative filter strips usually consider a limited number of factors (i.e. filter length, slope) and are in general based on empirical relationships. When an empirical approach is used, the application of the model is limited to those conditions of the data used for the regression equations.

The objective of this work is to provide a flexible numerical mechanistic tool to simulate dynamics of a wide range of surface runoff pollutants through dense vegetation and their physical, chemical and biological interactions based on equations defined by the user. This is the first time this approach has been used in vegetative filter strips. The ultimate goal of the model's flexibility is to help researchers and decision-makers estimate optimal filter characteristics (length, slope, vegetation) to achieve targeted runoff pollutant removal efficiency, while still considering the complex driving processes..

A flexible water quality model based on the Transport and Reaction Simulation Engine program (James, 2008b; Jawitz et al., 2008; James et al., 2009) is coupled to a transport module based on the traditional finite element method to solve the advection-

dispersion-reaction equation using the alternating split operator technique. This coupled model is linked to the VFSSMOD-W program (Muñoz-Carpena, 1993; Muñoz-Carpena et al., 1993a; Muñoz-Carpena et al., 1993b; Muñoz-Carpena et al., 1999; Muñoz-Carpena and Parsons, 2004; 2010) to mechanistically simulate mobile and stable pollutants through vegetative filter strips based on user-defined conceptual model where the pollutants and elements within the filter are expressed in terms of differential equations.

The numerical transport model was evaluated using analytical solutions and laboratory and field scale experiments. For the analytical testing, the water quality submodel performed well (Nash-Sutcliffe model efficiency coefficient > 0.99). The laboratory scale testing involved the simulation of bromide transport based on the exchange layer concept and the raindrop-induced chemical release theory (Gao et al., 2004). The model was able to explain the removal of bromide in runoff, but the incorporation of more processes is needed to give a more physically based explanation to the simulated results.

Field scale experimental testing involved the simulation of dissolved phosphorus in surface runoff, coming from phosphate mining tailing areas, through vegetative filter strips. The model helped to explain the dynamics of runoff dissolved phosphorus concentration through vegetative filter strips due to the dissolution of apatite (Kuo, 2007; Kuo and Muñoz-Carpena, 2009). The difference between the field data and the simulated data total mass of dissolved phosphorus concentration was less than 1%.

The incorporation of physically based theories to the flexible water quality module provides a useful tool to explain and predict the removal of runoff pollutants in

vegetative filter strips. Laboratory and field scale testing showed that the model can be applied to different conditions and scenarios.

One of the major advantages when using this tool is that the pollutant transport and removal through vegetative filter strips is related to physically based processes occurring within the filter. This mechanistic approach increases the range of use of the model when compared to the simplistic and limited empirical approach.

The use of more than one theory might be needed sometimes to simulate some pollutants. However, it is important to point out that the different theories to be used might not have additive properties, which could lead to the under or over estimation of the outflow concentration. The creation of a conceptual model that links how the pollutant interacts with the surrounding elements in the filter strip (i.e. grass, soil, sediments) is the key factor to consider in the flexible model. A poor conceptual model can lead to misunderstanding of the simulated results.

The potential uses and application of the model for different scenarios and pollutant models can help researchers, consultants, agencies or individuals to predict the amount of runoff pollutants that can be removed when vegetative filter strips are used. The strength of the model relies on the mechanistic approach used for simulating the removal of pollutants, and the flexibility of the model allows the user to apply current and future theories when analyzing the dynamics of pollutants in vegetative filter strips.

CHAPTER 1 INTRODUCTION

Today's natural resources are under threat. These threats are immediate as in the case of accidents (i.e. pollutant spills), and chronic as in the case of stormwater (which contains a wide range of pollutants, from eroded soil to fertilizer nutrients), complex organic chemical and pathogens, or diffuse pollution from automobiles and other sources across the landscape (Slawski, 2010). For many of these scenarios, the final fate of pollutants is the water bodies, where the pollutants could not only affect water quality but also ecosystem and human health. Chemicals can be transformed either in the source, during transport, or after the transport at the receiving site; however, nature has no permanent pollutants sinks. In this context, the so-called best management practices (BMP's) could be defined as means of promoting the capacity of pollutant sinks in terrestrial systems and of reducing the transfers of sinks to sources. Vegetative Filter Strips (VFS), which can be defined as (Dillaha et al., 1989) areas of vegetation designed to remove sediment and other pollutants from surface water runoff by filtration, deposition, infiltration, adsorption, absorption, decomposition, and volatilization, are a successful, natural, low-cost technology that has been used to reduce the load of sediments, nutrients, pesticides and even pathogens from non-point sources before it reaches a water body (rivers, ponds, etc) (Dooskey, 2001). They have been used especially in agricultural watersheds but also in construction, urban and forest environments.

Research about VFS during the last 20 years has focused on empirically assessing efficiencies for different pollutants and, in a few cases, on finding what mechanisms are involved in the removal process. The vegetative buffer length has been

commonly associated to its intended function. In this context, water bodies linked to wildlife habitats may need a buffer protection length of a couple of hundred of meters (Slawski, 2010). While tens of meters are typically sufficient to filter sediments, the effectiveness of VFS to reduce runoff pollutants (i.e. pesticides, nanoparticles, etc) relies not only in the length of the VFS, but also in various factors such as the type of soil, type of vegetation, slope, type of pollutant, sediment particle characteristics, amount of pollutant to retain in the VFS, among others. However, statistical analyses that attempt to relate physiographic characteristics of the VFS (i.e., slope and VFS length) to sediment and/or contaminant removal are the most common (Sabbagh et al., 2010).

Muñoz-Carpena et. al. (1993b; 1999; 2005) developed a physically based-mechanistic computer program based on the overland flow solution by Petrov-Galerkin Finite Elements Method called VFSSMOD-W (Muñoz-Carpena et al., 1993a), which simulates hydrology and sediment transport through vegetative filter strips on a storm-by-storm basis. In 2009, VFSSMOD-W incorporated a water quality module to estimate the removal efficiency of pesticides based on an empirical equation developed by Sabbagh et al. (2009). Recently, the US Environmental Protection Agency recognized to VFSSMOD-W as one of the recommended models that can be used to help to gather data and conduct data analyses to optimize VFS characteristics as a surface runoff pesticide control practice, and support quantification of pollutant loads and reductions (EPA, 2010). Recently, Sabbagh et al. (2010) proposed a revision of current pesticide EPA Tier II assessment during the registration process by introducing VFSSMOD-W as a component in the existing EPA modeling framework (PRZM/EXAMS).

Evaluating the removal of pollutants by considering the relevant mechanisms involved during their transport in runoff through VFS under dynamic conditions is desirable, since this approach is general and applicable to different pollutants and scenarios.

This document is divided into three papers that stand alone. Each paper focuses on a specific objective:

1. Development of a flexible numerical modeling component for surface runoff through dense vegetation and analytically testing for steady surface flow conditions.
2. Coupling of flexible surface runoff pollutant transport through dense vegetation component with a dynamic vegetative filter strip overland flow and sediment transport model (VFSSMOD-W) and testing with laboratory experimental data.
3. Field testing the dynamic model with experimental data from phosphorus mining tailing grass buffer plots.

CHAPTER 2
FLEXIBLE MODELING OF POLLUTANT TRANSPORT THROUGH DENSE
VEGETATION FOR STEADY SURFACE RUNOFF CONDITIONS

2.1 Introduction

The conservation of mass for a chemical that is transported either in surface or subsurface water can be driven by the 1-D Advection-Dispersion-Reaction Equation (ADR):

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2} - \Gamma(t) \quad (2-1)$$

Where C is the concentration of pollutant in water ($M T^{-3}$), t is time (T), v is (pore/surface) water flow velocity ($L T^{-1}$), x is distance (L), D_L is the hydrodynamic dispersion coefficient ($L^2 T^{-1}$), $D_L = D_m + \alpha_L v$, with D_m the molecular diffusion coefficient ($L^2 T^{-1}$), and α_L the longitudinal dispersivity (L). The term $-v \frac{\partial C}{\partial x}$ represents advective transport, $D_L \frac{\partial^2 C}{\partial x^2}$ represents dispersive transport, and $\Gamma(t)$ is the change in concentration due to reactions or as results of a source/sink element.

Substituting the elements of the hydrodynamic dispersion coefficient in (2-1),

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + (\alpha_L v + D_m) \frac{\partial^2 C}{\partial x^2} - \Gamma(t) \quad (2-2)$$

Analytical and numerical solutions have been proposed to solve the ADR.

Although the ADR is formally classified as a parabolic partial differential equation, if the advective term v dominates the diffusion/dispersion term D_L ($v \gg D_L$), it can become strongly hyperbolic. There are several analytical solutions to equation 2-1 (van Genuchten, 1982) that are rather limited in application because they are restricted to steady-state flow problems with regular boundaries (i.e. square domains) and constant coefficients (i.e. velocity, hydrodynamic dispersion). However, exact solutions are

important for validating and testing numerical models, and are used for this purpose in the testing sections 2.3 and 2.4.

Among numerical solutions, the finite difference method (FDM) and finite element method (FEM) are two of the most widely used schemes, but they are others methods that can be used (i.e random walk, method of characteristics). Finite-element method offers greater flexibility in special discretization than does the finites difference methods. For example, when using finite elements the domain can be discretized in irregular triangular elements for a better fitting of irregular boundaries in the domain. With the use of higher-order approximation, the FEM is generally more accurate than the standard FDM. Modification can be made to the FDM to reach the greater accuracy, but the simplicity related to these methods is lost (Zheng and Bennett, 2002).

Split operator (SO) approaches are popular for developing numerical algorithms to solve nonlinear, multicomponent, coupled reactive transport partial differential equations (PDEs) such as the ADR_{Re}Equation and for handling the different time scales of transport and reaction in the ADR (Morshed and Kaluarachchi, 1995; Barry et al., 1996a; Barry et al., 1996b; Barry et al., 1997; Barry et al., 2000; Simpson and Landman, 2008). These algorithms are constructed by separating each time integration step (of length Δt) into two substeps. First, the transport terms in the PDEs are integrated over Δt to yield an intermediate solution. Second, the transport and reaction processes are approximately coupled by integrating the reaction terms over Δt using the intermediate result as the initial condition.

From a practical perspective the most common question is which splitting method generates a better approximation: Transport first, then Reaction (TR), or Reaction first

then Transport (RT), or a combination of both such as Transport-Reaction-Transport (TRT) or Reaction-Transport-Reaction (RTR)? Simpson and Landman (2008) analyzed the temporal truncation error associated with TR, RT, and RTR. They concluded that the temporal truncation error is equal but opposite for TR and RT, which means that one overestimates and the other underestimates the solution. However, these authors found that the error can be removed with standard alternating SO schemes like TRT and RTR methods. Since the error produced is the same, both can be used to solve the ADR. Another question that arises regards the choice of the numerical method used for solving the ADR. Zheng and Bennett (2002) state that the finite element method is subject to the same numerical problems as the finite difference method, but with the use of higher-order approximations, the finite element method is more accurate than the finite difference method. It is also possible to use a higher-order approximation in the finite difference method. However, the simplicity of the method is lost. When the SO method is performed, the transport is solved with a finite difference/element method, and the reactive equation can be solved using an explicit method such as Runge-Kutta. However, if the system of equations exhibits a stiff behavior (i.e. rapid decay transient terms), an implicit method is recommended (James, 2008b).

Jawitz et al. (2008) and James (2008b; James et al., 2009) developed a novel program called Transport and Reaction Simulation Engine (TaRSE), for solving the 2-Dimensional ADR. The program solves the three parts—advective, dispersive, and reactive—of the equation independently, solving paired reaction and advection sub-steps symmetrically about the solution for the dispersive step. Although the program is stable for high Peclet numbers, it is the flexibility of the interface used for solving the

reactive part that makes this approach attractive and innovative for the simulation of transport and reaction of pollutants through VFS. In general, a user defined XML input file contains the mobile solutes (compounds to be transported and reacted), stable compounds (material that is not mobile, and is thus not transported but can react) and the different interactions among them. With this approach, the user not only has the control over the parameters, the types of reactions and the interaction among them, but can also define different levels of complexity based on research/management considerations and simplifications. However, for surface flow condition, a hydrodynamic model is required to supply TaRSE with the flow velocity and water depth data at each time step.

TaRSE was originally designed to run with the Regional Simulation Model (RSM) of the South Florida Water Management District (SFWMD) to evaluate the effects of different management scenarios in South Florida. The movement of phosphorus in the Florida Stormwater Treatment Area 1 West was the field test scenario used to demonstrate the high level of complexity that can be built using TaRSE (Jawitz et al., 2008). However, due to the ability of TaRSE to simulate a large flexible number of pollutants, current efforts are being focused to adapt TaRSE to other hydrodynamic programs such as SWIFT2D (Schaffranek, 2004) and in this current work with VFSSMOD (Muñoz-Carpena et al., 1999).

A new generic-flexible module to account for the transport and reaction of pollutants in surface runoff based on the solution of the 1-D ADR using a TRT SO method is presented here. This module combines a new standard Bubnov-Galerkin cubic/quadratic Finite Elements Method for solving the advective and dispersive

transport part of the 1-D ADR, with a flexible module that accounts for the reactive part of the ADR for single or multiple species. The reactive flexible module called Reaction Simulation Engine, RSE, is a windows library based on TaRSE, where the transport component has been removed. The resulting new module is called TRT, based on the Transport-Reaction-Transport sequence for numerically solving the ADR during each time step. The module is further tested under steady state conditions using conservative, first-order decay and Monod kinetics solutes..

2.2 Model Development

2.2.1 The Finite Elements Transport Module

In order to solve the ADR, we employ a standard Bubnov-Galerkin cubic/quadratic Finite Element Method for solving the spatial derivatives and a time-weighting (Crank-Nicholson) method for the temporal derivative (Miller, 1991).

The general form of the ADR for surface runoff is

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) - \vec{v} \cdot \nabla C + \left(\frac{\partial C}{\partial t} \right)_{\text{rxn}} + \Gamma(t) \quad (2-3)$$

where: C is the dissolved pollutant concentration; D is the hydrodynamic dispersion; \vec{v} is the average flow velocity, the subscript rxn denotes fluid-phase reactions (i.e. first order decay reaction); and $\Gamma(t)$ is a term to represent sources and sinks of the pollutant.

Equation (2-3) can be represented in one dimension, over the plane X, as follows:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) - v_x \frac{\partial C}{\partial x} + \left(\frac{\partial C}{\partial t} \right)_{\text{rxn}} + \Gamma(t) \quad (2-4)$$

When the sink/source term is not taken account, and we consider a first-order rate of degradation, equation (2-4) is transformed to

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) - v_x \frac{\partial C}{\partial x} - k_1 C \quad (2-5)$$

which can also be presented in operator notation

$$L(C) = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) - v_x \frac{\partial C}{\partial x} - k_1 C - \frac{\partial C}{\partial t} \quad (2-6)$$

Considering that when the method of weighted residuals is used, one equation exists for each node. The resultant system is then

$$\int_D W_i L(\hat{C}) dx = 0 \quad \text{for } i = 1, \dots, n_n \quad (2-7)$$

which can also be written as

$$\int_D W_i L(\hat{C}) dx = 0 \quad (2-8)$$

From Equation (2-8), the trial function can be defined as

$$\hat{C}(x) = \sum_{j=1}^{n_n} N_j(x) C_j \quad (2-9)$$

When using the Galerkin finite element method, equation (2-8) can be expressed as follows:

$$\int_D N_I L(\hat{C}) dx = 0 \quad (2-10)$$

By substituting the differential operator we have

$$\int_D N_I \left[\frac{\partial}{\partial x} \left(D_x \frac{\partial \hat{C}}{\partial x} \right) - v_x \frac{\partial \hat{C}}{\partial x} - k_1 \hat{C} - \frac{\partial \hat{C}}{\partial t} \right] dx = 0 \quad (2-11)$$

By separation of terms in Equation (2-11), we have

$$\int_D N_I \frac{\partial}{\partial x} \left(D_x \frac{\partial \hat{C}}{\partial x} \right) dx - \int_D N_I v_x \frac{\partial \hat{C}}{\partial x} dx - \int_D N_I k_1 \hat{C} dx - \int_D N_I \frac{\partial \hat{C}}{\partial t} dx = 0 \quad (2-12)$$

When the trial function is substituted in equation (2-12) we have

$$\begin{aligned}
& \int_D N_I \frac{\partial}{\partial x} \left[D_x \frac{\partial}{\partial x} \left(\sum_{j=1}^{n_n} N_j C_j \right) \right] dx - \int_D N_I v_x \frac{\partial}{\partial x} \left(\sum_{j=1}^{n_n} N_j C_j \right) dx \\
& - \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx - \int_D N_I \frac{\partial}{\partial t} \left(\sum_{j=1}^{n_n} N_j C_j \right) dx = 0
\end{aligned} \tag{2-13}$$

Equation (2-13) may be written as

$$\begin{aligned}
& \int_D N_I \frac{\partial}{\partial x} \left[D_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) \right] dx - \int_D N_I v_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx \\
& - \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx - \int_D N_I \frac{\partial}{\partial t} \left(\sum_{j=1}^{n_n} N_j C_j \right) dx = 0
\end{aligned} \tag{2-14}$$

Since the trial function is described with respect to spatial coordinates only, and the basis functions are not a function of time, equation (2-14) becomes

$$\begin{aligned}
& \int_D N_I \frac{\partial}{\partial x} \left[D_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) \right] dx - \int_D N_I v_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx \\
& - \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx - \int_D N_I \left(\sum_{j=1}^{n_n} N_j \frac{\partial C_j}{\partial t} \right) dx = 0
\end{aligned} \tag{2-15}$$

When the dispersive term is expanded we have:

$$\begin{aligned}
& \int_D N_I \frac{\partial D_x}{\partial x} \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx + \int_D N_I D_x \left(\sum_{j=1}^{n_n} \frac{d^2 N_j}{dx^2} C_j \right) dx \\
& - \int_D N_I v_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx - \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx \\
& - \int_D N_I \left(\sum_{j=1}^{n_n} N_j \frac{\partial C_j}{\partial t} \right) dx = 0
\end{aligned} \tag{2-16}$$

An approximation to Equation (2-16) can be obtained for the case when the spatial derivative of the hydrodynamic dispersion coefficient is small compared to the spatial derivative of concentration, as follows

$$\begin{aligned}
& \int_D N_I D_x \left(\sum_{j=1}^{n_n} \frac{d^2 N_j}{dx^2} C_j \right) dx - \int_D N_I v_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx \\
& - \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx - \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j \frac{\partial C_j}{\partial t} \right) dx = 0
\end{aligned} \tag{2-17}$$

If the basis functions are chosen to be C^0 continuous, the order of the derivative in the dispersive term—the first term—needs to be decreased from two to one. This may be accomplished using Green's theorem

$$\begin{aligned}
& \int_D N_I D_x \left(\sum_{j=1}^{n_n} \frac{d^2 N_j}{dx^2} C_j \right) dx \\
& = D_x N_I \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) \Big|_0^{x_L} - \int_D D_x \frac{dN_I}{dx} \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx
\end{aligned} \tag{2-18}$$

By combinations and reduction of similar terms of equations (2-17) and (2-18) we have:

$$\begin{aligned}
& \int_D D_x \frac{dN_I}{dx} \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx + \int_D N_I v_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx \\
& + \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx + \int_D N_I \left(\sum_{j=1}^{n_n} N_j \frac{\partial C_j}{\partial t} \right) dx \quad (2-19) \\
& = D_x N_I \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) \Big|_0^{x_L}
\end{aligned}$$

where the right-hand side of equation (2-19) represents a diffusive boundary flux. Since the diffusive boundary flux term is evaluated only on the boundary, and since this value is known for the case of natural or Newman boundary condition, equation (2-19) can be written in terms of the known value instead of the trial function

$$\begin{aligned}
& \int_D D_x \frac{dN_I}{dx} \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx + \int_D N_I v_x \left(\sum_{j=1}^{n_n} \frac{dN_j}{dx} C_j \right) dx \\
& + \int_D N_I k_1 \left(\sum_{j=1}^{n_n} N_j C_j \right) dx + \int_D N_I \left(\sum_{j=1}^{n_n} N_j \frac{\partial C_j}{\partial t} \right) dx \quad (2-20) \\
& = D_x N_I \frac{\partial C}{\partial x} \Big|_0^{x_L}
\end{aligned}$$

For the Dirichlet or necessary boundary conditions, the derivative is no longer known, but all references to the boundary node can be replaced with the known value – eliminating the equation from the system requiring solution.

In order to allow for parameter variation, it is convenient to integrate the left-hand side of equation (2-20) over the elements instead of the domain, which gives

$$\begin{aligned}
& \sum_{m=1}^{n_e} \left[\int_{\epsilon_m} D_x \frac{dN_I}{dx} \left(\sum_{j=1}^{n_m} \frac{dN_j}{dx} C_j \right) dx + \int_{\epsilon_m} N_I v_x \left(\sum_{j=1}^{n_m} \frac{dN_j}{dx} C_j \right) dx \right. \\
& \quad \left. + \int_{\epsilon_m} N_I k_1 \left(\sum_{j=1}^{n_m} N_j C_j \right) dx + \int_{\epsilon_m} N_I \left(\sum_{j=1}^{n_m} N_j \frac{\partial C_j}{\partial t} \right) dx \right] \quad (2-21) \\
& = D_x N_I \frac{\partial C}{\partial x} \Big|_0^{x_L}
\end{aligned}$$

where n_e is the total number of elements, and n_m is the number of nodes in the element m .

By applying finite difference approximation to solve the derivative in time in Equation (2-21):

$$\begin{aligned}
& \sum_{m=1}^{n_e} \left[\int_{\epsilon_m} D_x \frac{dN_I}{dx} \left(\sum_{j=1}^{n_m} \frac{dN_j}{dx} C_j^{l+1} \right) dx + \int_{\epsilon_m} N_I v_x \left(\sum_{j=1}^{n_m} \frac{dN_j}{dx} C_j^{l+1} \right) dx \right. \\
& \quad \left. + \int_{\epsilon_m} N_I k_1 \left(\sum_{j=1}^{n_m} N_j C_j^{l+1} \right) dx \right. \quad (2-22) \\
& \quad \left. + \int_{\epsilon_m} N_I \left(\sum_{j=1}^{n_m} N_j \frac{C_j^{l+1} - C_j^l}{\Delta t} \right) dx \right] = D_x N_I \left(\frac{\partial C}{\partial x} \right)^{l+1} \Big|_0^{x_L}
\end{aligned}$$

which can also be expressed as

$$\begin{aligned}
& \sum_{m=1}^{n_e} \left[\int_{\varepsilon_m} D_x \frac{dN_I}{dx} \left(\sum_{j=1}^{n_m} \frac{dN_j}{dx} C_j^{l+1} \right) dx + \int_{\varepsilon_m} N_I v_x \left(\sum_{j=1}^{n_m} \frac{dN_j}{dx} C_j^{l+1} \right) dx \right. \\
& \quad \left. + \int_{\varepsilon_m} N_I k_1 \left(\sum_{j=1}^{n_m} N_j C_j^{l+1} \right) dx + \int_{\varepsilon_m} N_I \left(\sum_{j=1}^{n_m} N_j \frac{C_j^{l+1}}{\Delta t} \right) dx \right] \quad (2-23) \\
& = \sum_{m=1}^{n_e} \left[\int_{\varepsilon_m} N_I \left(\sum_{j=1}^{n_m} N_j \frac{C_j^l}{\Delta t} \right) dx \right] + D_x N_I \left(\frac{\partial C}{\partial x} \right)^{l+1} \Big|_0^{x_L}
\end{aligned}$$

where time step l is the known time level and $l+1$ is the time traveled sought. By writing Equation (2-23) in matrix notation we have:

$$\begin{aligned}
& \sum_{m=1}^{n_e} ([A_D^m \{C^m\}^{l+1}] + A_v^m \{C^m\}^{l+1} + A_k^m \{C^m\}^{l+1} + A_t^m \{C^m\}^{l+1}) \\
& = \sum_{m=1}^{n_e} (A_t^m \{C^m\}^l) + \{b_D\} \quad (2-24)
\end{aligned}$$

Where $[A_D]$ is the hydrodynamic dispersion coefficient matrix, $[A_v]$ is the velocity coefficient matrix, $[A_k]$ is the reaction coefficient matrix, $[A_t]$ is the temporal coefficient matrix –all corresponding to the appropriate integral terms in equation (2-24) and all are defined over an element; and $\{b_D\}$ is a dispersive boundary-flux vector.

At the end, the application of the finite element method results in a system of linear equations which need to be solved. This number of equations is a function of the number of nodes and the nodal degrees of freedom. In this program, called TR-FEM (fully coupled Transport-Reaction model using Finite Elements Method), the solution can be simplified in the next steps:

1. Form the system matrix $[A]$ of constant coefficients
2. Perform LU decomposition over this matrix $[A]$
3. Form the system matrix $[BM]$ of constant coefficients

4. Form the right hand side of equation (vector $\{b\}=[BM]\{X\}$ for each time step
5. Solve for $[A],\{b\}$ to get $\{X\}$, the vector with the concentrations.
6. Repeat 4 & 5 until completion of desired number of time steps

Where $[A]$ is a square, $N \times N$ system matrix, $\{b\}$ is the $1 \times N$ right hand side vector, and $\{X\}$ is the $1 \times N$ solution vector at time step $t+1$.

The TR-FEM program assumes steady state flow conditions. This means that the flow velocity, flow depth and the hydrodynamic dispersion coefficient are considered as constant during the entire simulation. The program was tested for analytical solutions to four different scenarios: 1) a constant pollutant flow (a constant pollutant concentration is released at the first node of the domain during the entire simulation), 2) a pollutant plug flow (a pollutant of constant concentration is released in the first node for a specific time, which is less than the total time of the simulation), 3) a time dependent flow (the pollutant is released in the first node of the domain during the entire simulation, where the concentration released is based on a time dependent function and 4) a non-advective example using Monod kinetics based on the work of (Simpson and Landman, 2007).

TR-FEM can be run for transport only, or for transport and reaction, depending on the value of the first order decay coefficient k_1 (Equation 2-5). When compared to analytical solutions, the fully coupled TR-FEM yields a better approximation to the analytical solution when compared to ordinary split operator methods and a similar accuracy level with the alternating TRT SO method (section 2.4.1 and 2.4.2).

When no analytical solution is available, such as with the Monod Kinetics (Simpson and Landman, 2007), the TR-FEM scheme is used as an “analytical solution” in order to compare it with the TR and TRT split operator methods.

In general, the input data parameters needed to run TR-FEM correspond to those for the numerical discretization (spatial domain and time step), flow velocity, hydrodynamic dispersivity, and coefficient of reaction if applicable. Details on the program input file and examples are given in Table A-1 in Appendix A.

2.2.2 The Reactive Module

James et al. (2009) presented a 2-Dimensional spatially distributed numerical component for simulating water quality within the South Florida Water Management District Regional Simulation Model (RSM). RSM simulates surface-water and ground-water hydrodynamics on an unstructured triangular mesh using the Hydrologic Simulation Engine (HSE), which implements a finite-volume method to calculate water heads and flows. The component developed by James et al. (2009), called Transport and Reaction Simulation Engine (TaRSE), was linked to RSM to simulate transport and reaction of pollutants in a constructed wetland in South Florida.

TaRSE numerically approximates the solution to the 2D advection-dispersion-reaction equation. It treats the three processes of the 2-D ADR (advection, dispersion and reaction) independently. The reactive step solves a coupled system of ordinary differential equations (ODE) describing the interaction between the simulated reactive components (i.e. solute-soil, porewater-soil, etc). The solution to the system of ODE is based on the fourth-order Runge-Kutta method (RK4), which provides a $O(\Delta t^5)$ local error and a $O(\Delta t^4)$ global error during the simulation. RSE does not solve the hydrodynamic equations; and relies on a separate hydrodynamic model to obtain the flow between spatial elements (James et al., 2009).

Jawitz et al. (2008) presented and tested the transport of phosphorus in wetlands based on the interactions between stores and components using TaRSE. A component is defined in TaRSE as a variable that is of interest of the user (i.e. phosphorus, nitrogen, oxygen, etc), or it can also be a parameter that is sometimes useful to describe a specific reaction (i.e. dispersion coefficients, sorption and desorption coefficients, etc). Variables can be classified into two types: mobile variables, which are transported by water or some other mechanism (i.e. dissolved pollutants in surface water), and stable variables, which are stationary in the domain (sorbed pollutant to soil). Stores hold the various components, and these components (i.e. dissolved phosphorus) are transported between stores by flow. A given store can hold both mobile and stable variables, as well as parameters and variables. Variables cannot be moved from element to element. An example of stores can be the surface water, which can hold different pollutants, and soil which holds porewater and the soil matrix with different chemical elements in it (Figure 2-1).

The model allows adding stores and elements in order to increase the level of analysis and complexity of the system. Originally, TaRSE was tested using three user-defined levels of complexity to simulate the transport of phosphorus in wetlands (Figure 2-2). The first level of complexity included the adsorption-desorption process of phosphorus from the water column to the porewater and the incorporation of phosphorus from the soil matrix to the porewater. The second level of complexity added plankton to the water column, which interacted with the soluble P and the soil. The third level included plankton and macrophytes, which consume soluble P from the water column and the porewater.

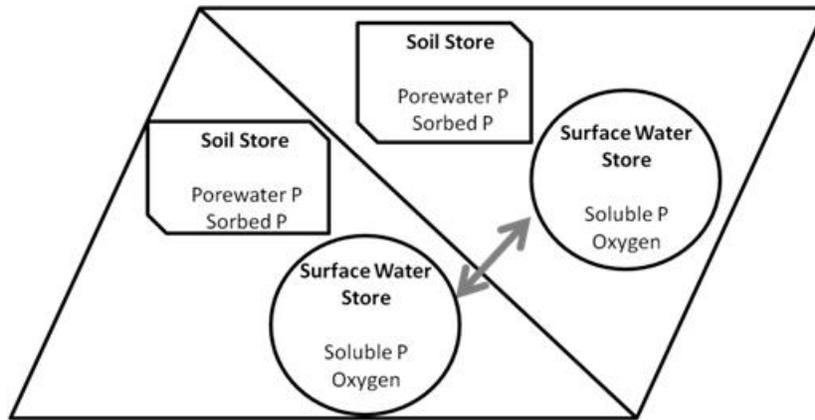


Figure 2-1. Simple 2-D conceptual movement of mobile and stable components between two triangular elements (cells) in TaRSE. Mobile components soluble P and oxygen are transported with the flow from one element to the other. Stable components porewater P and sorbed P can interact (react) with mobile components but cannot be transported between elements. P stands for pollutant.

TaRSE uses the XML format to define the relationships between the different components in equations. Each equation consists of a left-hand side (lhs) that contains the name of the variable to which the equation is applied, and a right-hand (rhs) side that contains the equation in a string. Each equation is an ordinary differential equation with respect to time that describes how the particular left-hand side variable evolves with time. The string that defines the right-hand side of the equation is parsed by TaRSE to create a function that is evaluated by the fourth order Runge Kutta method to solve the differential equation. As an example, Figure 2-3 shows the interactions between two variables named `water_column_p` representing phosphorus in the water column (C_w) and `settled_p` representing settled phosphorus (C_s), and two reaction coefficients k_u and k_r based on a simple uptake/release model.

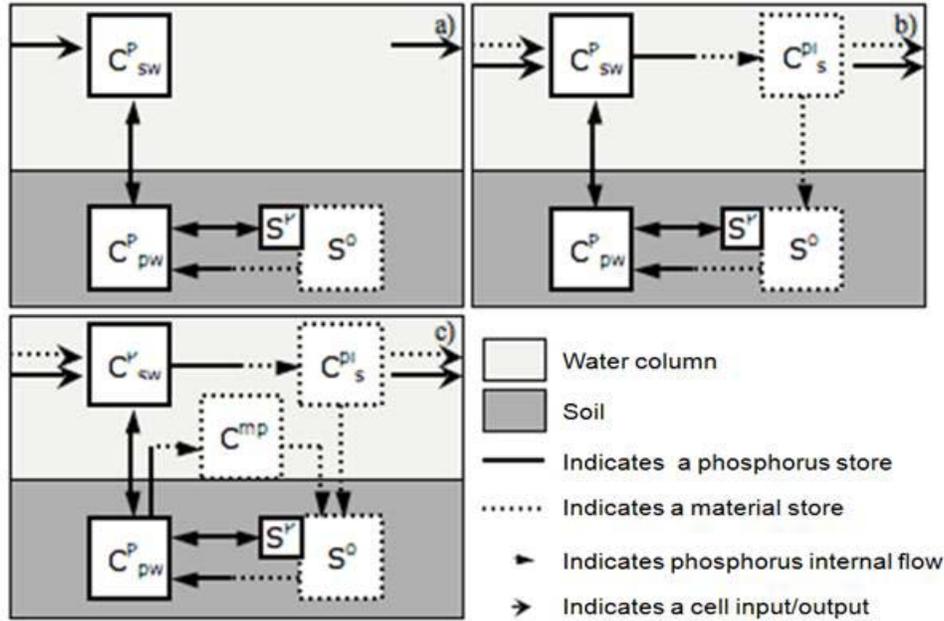


Figure 2-2. Conceptual model for complexity levels 1 (a), 2 (b) and 3 (c) showing different phosphorus interactions among surface water, porewater, plankton and macrophytes. C_{sw}^P is surface water SRP, C_{pw}^P is soil porewater SRP, S^P is soil adsorbed phosphorus, S^o organic soil, C_s^{pl} is plankton biomass and C^{mp} is macrophyte biomass. SRP is soluble reactive phosphorus. Source: Adapted from Jawitz et al. (2008)

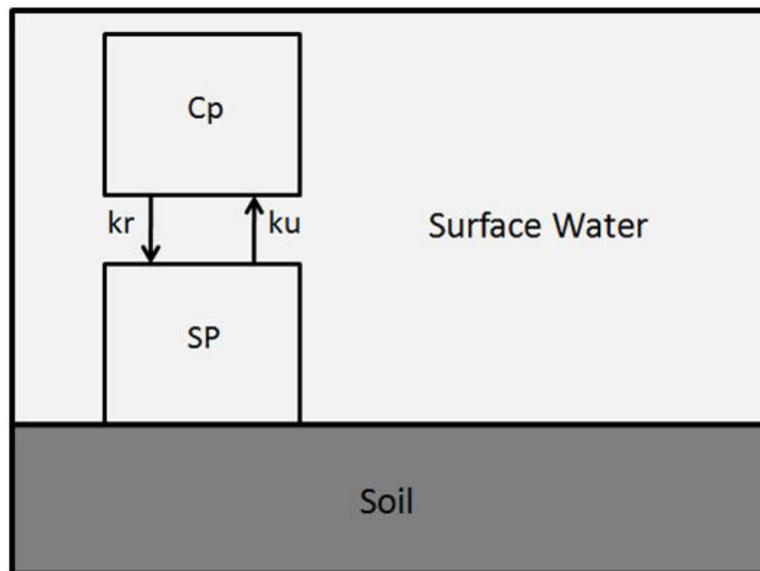


Figure 2-3. Basic conceptual model for uptake/release dynamics of phosphorus between the soluble phosphorus in water column and settled phosphorus on soil. Source: Adapted from James (2008b).

The phosphorus interactions depicted in Figure 2-3 can be written by equations (2-25) and (2-26) as follows:

$$\frac{dC_w}{dt} = -k_u C_w + k_r C_s \quad (2-25)$$

$$\frac{dC_s}{dt} = k_u C_w - k_r C_s \quad (2-26)$$

This system of equations would be written in the TaRSE XML input file as shown in Table A-2 in Appendix A.

Since VFSSMOD is based on a 1-D effective (2-D averaged) finite element method for simulation of surface runoff in filter strips, a modified version of TaRSE suitable for 1-Dimensional domain was needed. James (2008ab) prepared a modified version of TaRSE for coupling it to other programs. This adapted version, called Reaction Simulation Engine (RSE), handles the reactive component suitable for any type of dimensional problem, while relies on transport component provided by another program. RSE is called as a library for a program that handles the hydrodynamic (flow velocity, water depth, etc) and transport processes. The Reaction Simulation Engine keeps all the features of TaRSE for handling an unlimited number of compounds and their interactions. Table A-3 (Appendix A) contains the details on the input sections needed to run the XML input file in RSE.

2.2.3 Linkage between Transport and Reaction Components – Split Operator

Based on the work developed by Kaluarachchi and Morshed, 1995; Morshed and Kaluarachchi, 1995; Simpson and Landman, 2007, the traditional split operators TR and RT have greater errors when used to approximate the ADR compared to the alternating TRT and RTR split operators. In a problem with a single species Monod decay, Simpson and Landman (2007) have shown that the RT overestimates the solution and

TR underestimates in the same proportion, meanwhile TRT and RTR showed no visual difference with the solution presented.

Simpson and Landman (2008), stated that implementing alternating split operator methods can be problematic since the $O(\Delta t)$ temporal truncation error (TTE) is only removed after taking an even number of time steps. This can be explained as follows: since the TTE associated with TR splitting is equal and opposite to the TTE associated with RT splitting, then for sufficiently small Δt , the $O(\Delta t)$ TTE incurred in one time step will be removed by reversing the sequential order of splitting in the following step. This will lead to the $O(\Delta t)$ TTE being removed after every second (even) time step. Two methods are proposed in order to deal with the TTE:

1. Within each time step, a TRT alternating algorithm solves first the transport for $\Delta t/2$ then the reaction for Δt and another transport for $\Delta t/2$.
2. Within each time step, an RTR alternating algorithm solves first the reaction for $\Delta t/2$ then transport for Δt and another reaction for $\Delta t/2$.

The fully coupled TR-FEM and RSE were linked first as a TR split operator where TR-FEM solves the transport and RSE the reactive process of ADR. This module is called TR-RSE.

For the alternating split operator method, the TRT sequence was used because RSE is a program that is computationally more expensive than the fully coupled TR-FEM, so the sequence RTR is more expensive. Different combinations of temporal and spatial steps were analyzed in order to evaluate how they affect the time needed to complete the simulation. The alternating RTR split operator method was not tested in this work because of the high computational cost.

The following combinations were chosen to be tested with and without a reactive term:

- TR-FEM: The solution to the ADR is based on the fully coupled (Transport-Reaction) finite elements method.
- TR-RSE: A TR split operator method used to solve the ADR. Transport is solved using the finite elements method component of TR-FEM, and the reaction(s) is solved with RSE.
- TRT: An alternating split operator method TRT is used to solve the ADR during each time step. Transport is solved using the finite elements method, and the reaction(s) is solved with RSE.

Details of program implementation of these alternatives are given in Appendix A (Tables A-4 and A-4).

2.3 Model Testing

The programs TR-FEM, TR-RSE and TRT were tested with four different scenarios using conservative and reactive conditions for a total of seven scenarios: 3 conservative and 4 reactive (see in Table 2-1). The four scenarios used are:

Scenario I: A continuous and constant inflow of pollutant

Scenario II: A plug of pollutant released during 1 minute.

Scenario III: A continuous and variable input of pollutant as a function of time (pollutant concentration changes with time).

Scenario IV: Dispersion of a pollutant in a no-flow solution domain and reaction based on Monod kinetics.

Scenarios I, II and III were tested with two conditions: a) the pollutant is a conservative tracer and b) the pollutant is transported and reacted based on first order decay kinetics. A schematic representation of scenarios I, II and III is shown in Figure 2-4, where runoff is running over an impermeable surface of 20 m length. An arbitrary pollutant is injected at $x=0$ m and $t=0$ min, following the different scenarios depicted in Table 2-1.

Table 2-1. Scenarios used to test the programs TR-FEM, TR-RSE and TRT

Scenario	L (m)	Xo (m) +	V (m/s)	DL (α_L, D_m) (m^2/s) (m, m^2/s)	dx (m)	dt (s)	Lateral inflow Co (g/m^3)	t _{end} (s)	Reaction	C _i initial condition (t=0) (g/m^3)
I. Constant lateral inflow of pollutant in runoff	20	10	0.166	0.0167 (0.099,0.01)	0.1	1.66x10 ⁻⁴ 8.33x10 ⁻⁴ 4.16x10 ⁻⁴	100; t>0	150	k ₁ = 0*; k ₁ =0.1**	0, $\forall x$
II. Lateral plug of pollutant in runoff	20	10	0.166	0.0167 (0.099,0.01)	0.1	1.66x10 ⁻⁴ 8.33x10 ⁻⁴ 4.16x10 ⁻⁴	100; 0<t<60s	180	k ₁ = 0*; k ₁ =0.1**	0, $\forall x$
III. Variable continuous lateral inflow of pollutant in runoff	20	10	0.166	0.0167 (0.099,0.01)	0.1	1.66x10 ⁻⁴ 8.33x10 ⁻⁴ 4.16x10 ⁻⁴	80+30e ^{-t} 0<t<t _{end}	180	k ₁ = 0*; k ₁ =0.1**	0, $\forall x$
IV. Dispersion of Monod reactive pollutant in No-Flow domain (Simpson and Landman, 2007)	30	20 -30	0	1 (0,1)	0.01	0.05	0	1	$\alpha_m=1$; k _m =0.1	e ^{-(x-15)^2}

* Conservative

** Reactive

k₁: First order reaction kinetics constant, s-1

α_m, k_m : Monod decay constants

+: Observation point

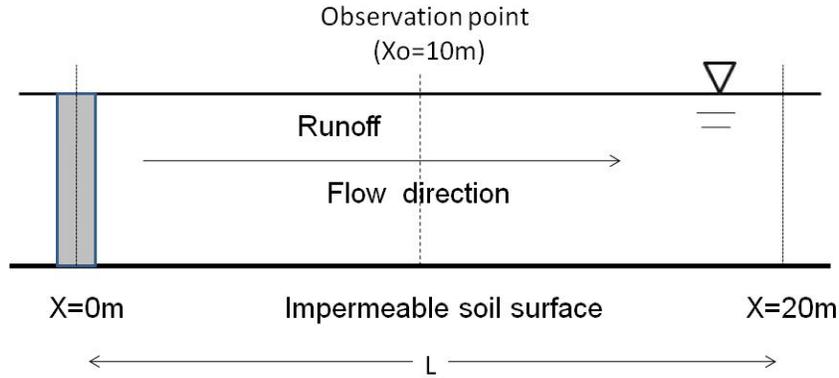


Figure 2-4. Schematic representation of the scenarios used to test TR-FEM, TR-RSE and TRT programs.

For scenarios I, II and III, stability and accuracy of the simulations were controlled by choosing a fixed value of the Peclet number of 1 and three different values of the Courant number less than or equal to 1 (0.25, 0.5 and 1).

The fourth scenario is based on the work developed by Simpson & Landman (2007), where a pollutant is initially distributed over the domain at $t=0$ as stated in Table 2-1. For this scenario, the pollutant is degraded over the domain, without transport, based on Monod kinetics. Since no analytical solution exists for Monod kinetics, the results from Simpson & Landman (2007) were compared with those obtained with the models developed herein for evaluation purposes.

2.3.1 TR-FEM Transport Model Testing

Scenarios I, II and III were tested using the analytical solutions reported by van Genuchten (1982). For scenarios I and II, the governing equation for a conservative solute is given by:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (2-27)$$

with the next initial and boundary conditions

$$C(x,0)=C_i=0$$

$$C(0,t) = \begin{cases} C_0 & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

When a continuous input of pollutant is tested, t_0 is assumed to be the total time of simulation.

When scenario III is tested, equation (2-27) has the next initial and boundary conditions for a conservative solute:

$$C(x,0) = C_i = 0$$

$$C(0,t) = C_a + C_b e^{-\lambda t} \quad \text{with } C_a=80, C_b=30 \text{ and } \lambda=1$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

The full analytical solution for conservative solute transport for each one of the first three scenarios is presented in Appendix A.

For the case of transport of a solute with a first order reactive term, the governing equation given by van Genuchten (1982) is:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \mu C + \gamma \quad (2-28)$$

with $\mu=0.1$ and $\gamma=0$.

With the same initial and boundary conditions used for the conservative solute.

The analytical solution for each one of the three reactive first order decay scenarios is presented in detail in Appendix A.

The L^2 error norm was calculated for the first three scenarios using the simulated data and the analytical solution.

The parameters used to test the fully coupled transport-reaction finite elements method were: total length (domain): 20 m, flow velocity: 0.1667 m/s, hydrodynamic dispersion coefficient D_L : 0.0167 m²/s (combining the longitudinal dispersivity $\alpha_L=0.099$ m and the molecular the diffusion coefficient $D_m=1.66 \times 10^{-4}$ m²/s (for the given velocity) and, spatial step dx: 0.1 m. The program was evaluated using three different time steps: 0.6, 0.3 and 0.15 seconds.

For the first scenario, a pollutant of concentration $C_o=100$ g/m³ is released during the entire time of the simulation at $t=0$ min and $x=0$ m. Time of simulation was set to 150 seconds. The concentration was reported at the middle of the domain.

For the second scenario, a plug of pollutant with concentration $C_o=100$ g/m³ is released for one minute at $x=0$ m and $t=0$ min. Time of simulation was set to 180 seconds. The concentration was reported at the middle of the domain.

For the third scenario, a pollutant is released continuously at $x=0$ m and time= 0 min. The concentration changes in time based on the expression $C_o=80+30 \cdot \exp(-t)$ [g/m³]. Time of simulation was set to 3.0 min. The concentration was reported at the middle of the domain.

The fourth scenario was not used to evaluate the transport module because the pollutant was not transported in the domain; it only was diffused from the soil to the water column. However, this scenario was used to test the split operator methods TR-RSE and TRT. The Nash-Sutcliffe coefficient was used to estimate the difference between the simulated results by using TR-RSE and TRT and those values reported by Simpson and Landman (2007).

2.3.2 Coupled TR-RSE and TRT Split Operator Methods Testing

The split operator TR-RSE and TRT programs were tested following the same scenarios depicted in this section but including a reactive term based on a first order decay kinetics with a value of 0.1 min^{-1} for the decay coefficient. The advective and dispersive part of the ADR (Eq. 2-2) is solved using the TR-FEM program. After the pollutant has been transported, the reactive (decay) term is solved using RSE. The differential equation to be used for the reactive term can be written as follows:

$$\frac{dC}{dt} = -k_1 C \quad (2-29)$$

where C is the pollutant concentration in the water column (runoff) and k_1 is the first order decay coefficient.

Equation (2-23) can be written in the XML input file as follows:

```
<equations>
  <equation>
    <lhs>water_column_p</lhs>
    <rhs>k1*water_column_p</rhs>
  </equation>
</equations>
```

An additional input file (*.iwq) with the parameters to be used is needed. This file is detailed in Table A-5, where only one mobile variable called water_column_p, no stable element and one parameter (k_1) are used in the simulation. This information has to be included in the corresponding XML input file (see Appendix A).

In order to test TR-RSE and TRT with the fourth scenario (Monod kinetics), the procedure depicted in Simpson and Landman (2007) was used. In this example, an initial amount of some pollutant is distributed in the domain, at $t=0$, based on the following expression:

$$C(x, 0) = e^{-(x-25)^2} \quad (2-30)$$

The transport of the pollutant is considered to be only dispersive (no flow), and the reaction follows Monod kinetics

$$\frac{dC}{dt} = \frac{\alpha C}{K + C} \quad (2-31)$$

All results were evaluated using $dx = 0.01$ and $dt = 0.05$. The decay parameters are $\alpha = 1$ and $K = 0.1$. The diffusion coefficient was $D = 1$. Results of the simulation were compared visually with those reported by Simpson and Landman (2007), where units are not reported, but considered to be consistent.

2.4 Results

2.4.1 Non-Reactive Scenarios

Scenarios I, II and III were used to test the transport of a pollutant using the fully coupled TR Finite Elements Method without the sink/source element $\Gamma(t)$. Since the transport modules of TR-RSE and TRT split operator methods are based on TR-FEM, results can be shown together in Table 2-2 and Figures 2-5, 2-6 and 2-7.

All the scenarios are compared visually and numerically with the analytical solutions (van Genuchten, 1982).

Table 2-2. Comparison of models TRT, TR-FEM and TR-RSE based on L^2 error norm, for non-reactive scenarios using different values of dt and courant number. Peclet number was set to 1 for all scenarios. Global results shows efficiency reached for the entire domain at the end of simulation. Local domain shows efficiency reached for the most critical part of the fitting curves, which is for the interval 66 - 90 seconds for scenario I; from 71 to 108 seconds for scenario II and from 71 to 96 seconds for scenario III.

Scenario	Method	Courant Number, CN	Time step, dt (s)	Global L^2 error norm	Local L^2 error norm
I. Continuous (Non-Reactive)	TR-RSE	1	0.6	7.45	2.59
		0.5	0.3	5.15	1.80
		0.25	0.15	3.60	1.26
	TR-FEM	1	0.6	7.45	2.59
		0.5	0.3	5.15	1.80
		0.25	0.15	3.60	1.26
	TRT	1	0.6	3.64	1.29
		0.5	0.3	2.55	0.90
		0.25	0.15	1.79	0.63
II. Plug (Non-Reactive)	TR-RSE	1	0.6	10.53	1.49
		0.5	0.3	7.28	1.10
		0.25	0.15	5.09	0.80
	TR-FEM	1	0.6	10.53	1.49
		0.5	0.3	7.28	1.10
		0.25	0.15	5.09	0.80
	TRT	1	0.6	5.15	0.80
		0.5	0.3	3.60	0.57
		0.25	0.15	2.53	0.41
III. Variable injection (Non-Reactive)	TR-RSE	1	0.6	8.19	1.33
		0.5	0.3	5.66	0.96
		0.25	0.15	3.96	0.69
	TR-FEM	1	0.6	8.19	1.33
		0.5	0.3	5.66	0.96
		0.25	0.15	3.96	0.69
	TRT	1	0.6	4.00	0.70
		0.5	0.3	2.80	0.49
		0.25	0.15	1.97	0.35

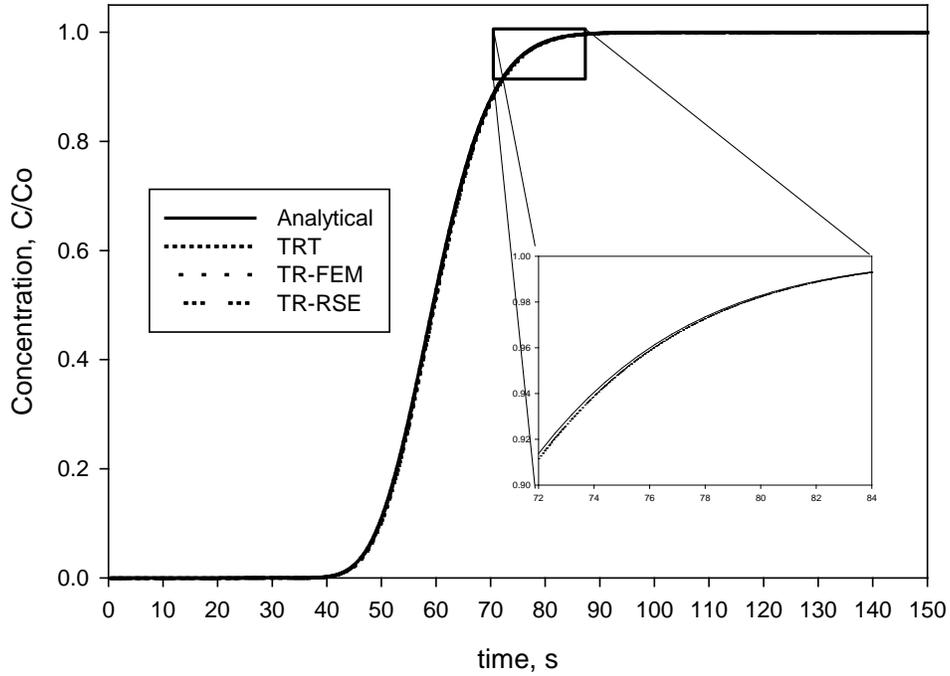


Figure 2-5. Comparison for ADR solution at $x=10$ m (half of the domain) for continuous input of conservative pollutant (Scenario I, Table 1-1)

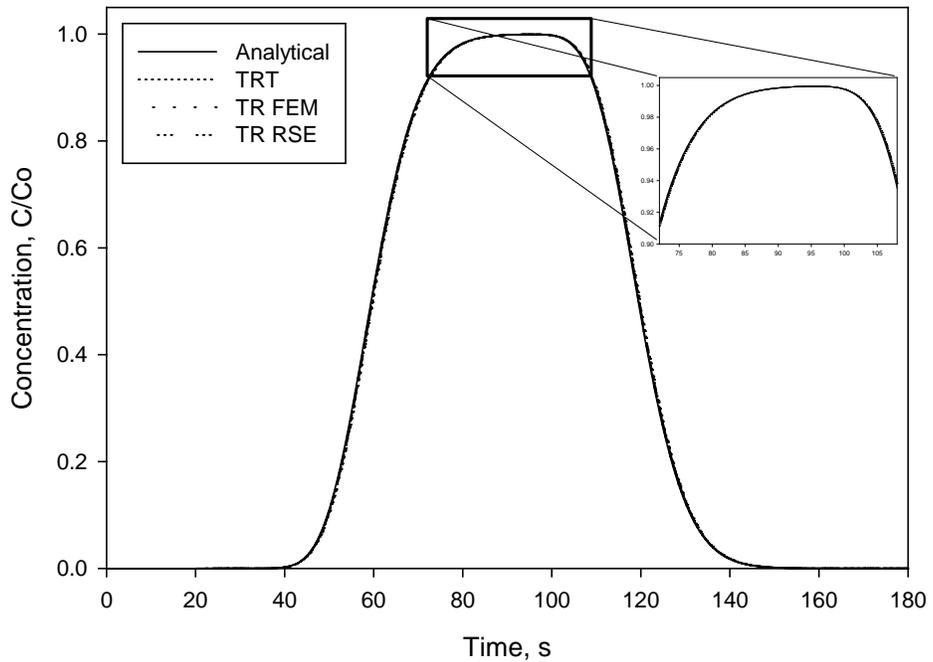


Figure 2-6. Comparison for ADR solution at $x=10$ m (half of the domain) for a plug of a conservative pollutant (Scenario II, Table 1-1).

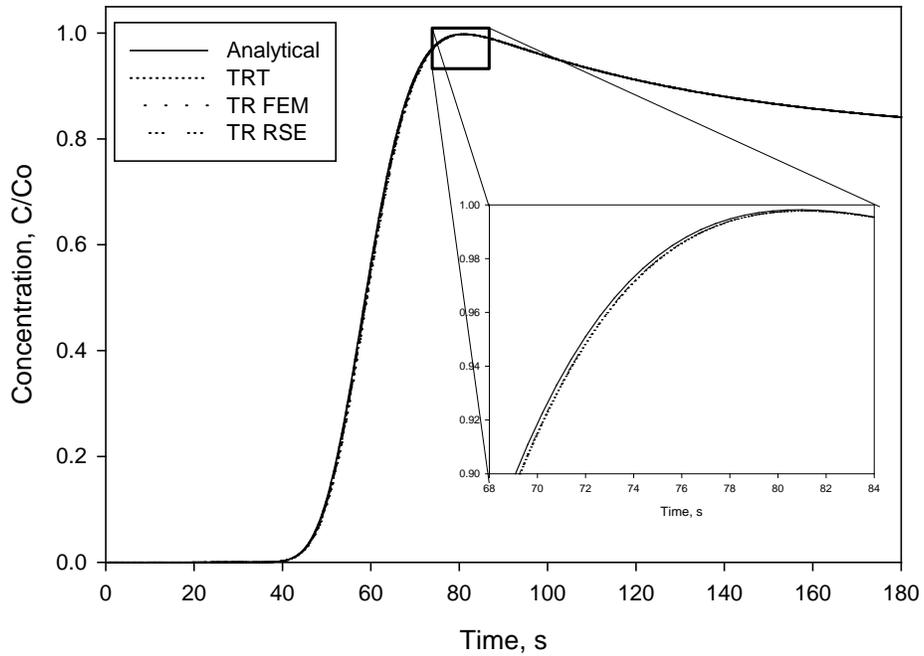


Figure 2-7. Comparison for ADR solution at $x=10$ m (half of the domain) for a variable time dependant input of conservative pollutant (Scenario III, Table 1-1)

2.4.2 Reactive Scenarios

Once RSE was evaluated with two different scenarios (see RSE Reactive Module Testing Section in Appendix A for more details), the coupled programs TR-FEM, TR-RSE and TRT were evaluated for a first order decay and Monod kinetics reactions. Results of the simulations are shown in Table 2-3 and Figures 2-8, 2-9, 2-10 and 2-11.

Table 2-3. Comparison of models TRT, TR-FEM and TR-RSE based on L2 error norm, for reactive scenarios using different values of dt and courant number. Peclet number was set to 1 for all scenarios. Global results shows efficiency reached for the entire domain at the end of simulation. Local domain shows efficiency reached for the most critical part of the fitting curves, which is for the interval 66 – 90 seconds for scenario I; from 71 to 108 min for scenario II and, from 76 to 96 min for scenario III.

Scenario	Method	Courant Number, CN	Time step, dt (s)	Global L ² error norm	Local L ² error norm
I. Continuous (Reactive)	TR-RSE	1	0.6	6.91	2.48
		0.5	0.3	4.78	1.72
		0.25	0.15	3.33	1.20
	TR-FEM	1	0.6	6.75	2.30
		0.5	0.3	4.67	1.60
		0.25	0.15	3.26	1.12
	TRT	1	0.6	3.29	1.15
		0.5	0.3	2.30	0.79
		0.25	0.15	1.61	0.54
II. Plug (Reactive)	TR-RSE	1	0.6	9.55	1.44
		0.5	0.3	6.61	1.05
		0.25	0.15	4.62	0.75
	TR-FEM	1	0.6	9.54	1.34
		0.5	0.3	6.60	0.99
		0.25	0.15	4.62	0.72
	TRT	1	0.6	4.67	0.72
		0.5	0.3	3.27	0.51
		0.25	0.15	2.30	0.36
III. Function (Reactive)	TR-RSE	1	0.6	7.59	1.36
		0.5	0.3	5.25	0.98
		0.25	0.15	3.66	0.69
	TR-FEM	1	0.6	7.42	1.17
		0.5	0.3	5.13	0.85
		0.25	0.15	3.59	0.61
	TRT	1	0.6	3.62	0.61
		0.5	0.3	2.53	0.42
		0.25	0.15	1.77	0.29
IV Monod kinetics	TRT	-	0.05	0.9993*	0.9893*
	TR-RSE	-	0.05	0.9862*	0.7036*

* Nash-Sutcliffe coefficient.

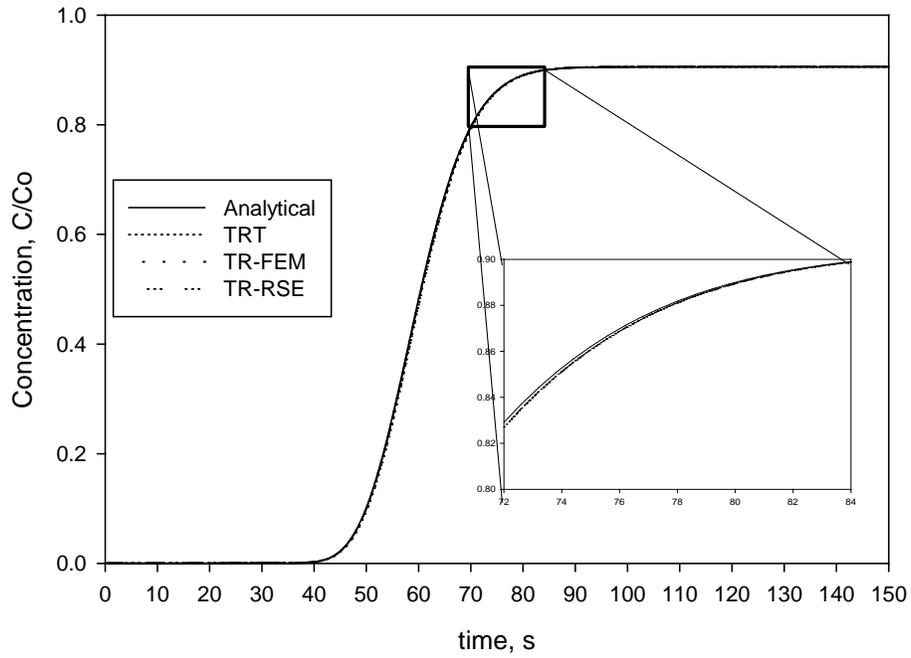


Figure 2-8. Comparison for ADR solution at $x=10$ m (half of the domain) for continuous input of pollutant with reactive term (Scenario I, Table 2-1)

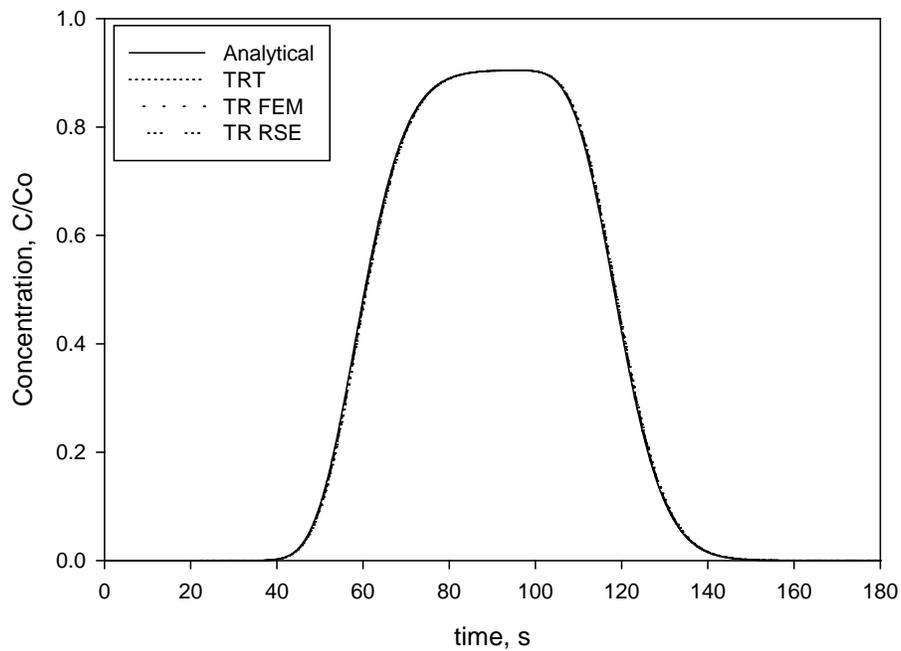


Figure 2-9. Comparison for ADR solution at $x=10$ m (half of the domain) for a plug of a pollutant with reactive term (Scenario II, Table 2-1)

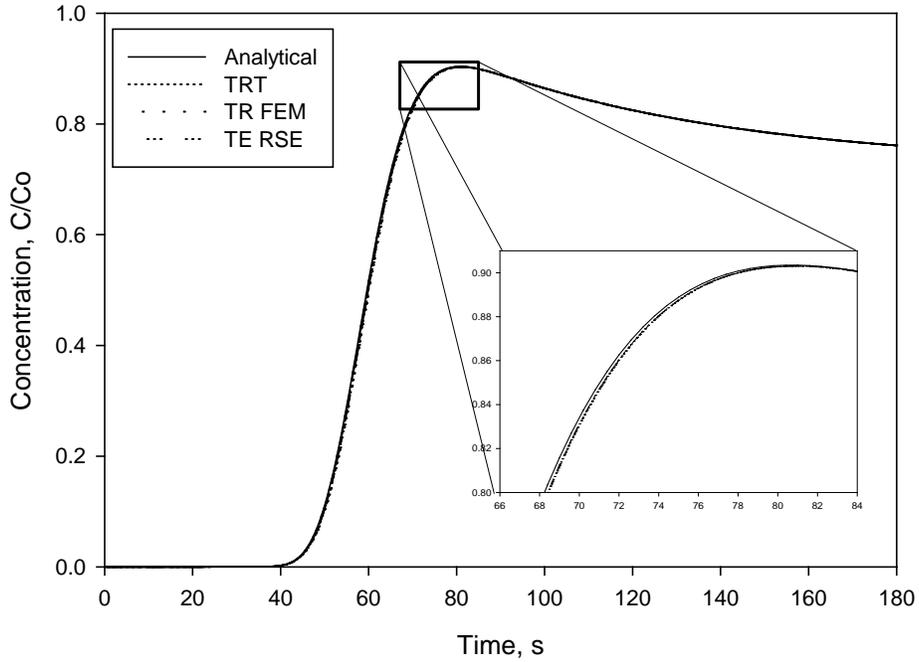


Figure 2-10. Comparison for ADR solution at $x=10$ m (half of the domain) for a variable time dependant input of pollutant with reactive term (Scenario III, Table 2-1)

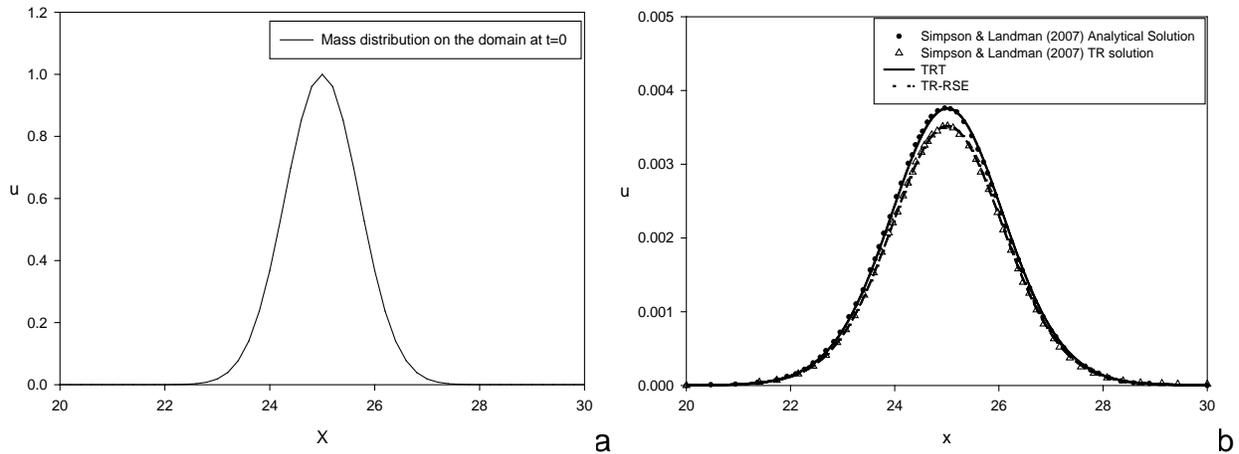


Figure 2-11. Pollutant Mass distribution at $t=0$ (a) and (b) comparison between the modules TRT (split operator) and TR-RSE with the results obtained by Simpson and Landman (2007) for Monod kinetics (Scenario IV, Table 2-1).

Mass balance results for a conservative pollutant under scenario II and for a reactive pollutant under scenarios II and IV can be found in Table 2-4, where the total input mass is compared to the different solution presented in this chapter.

Table 4-4. Mass balances for scenarios II and IV.

Scenario	Input	Analytical	TRT	TR-FEM	TR-RSE
Conservative pollutant					
Scenario II (Plug), g	1000	1000	1000.003	999.996	999.996
Reactive pollutant					
Scenario II (Plug), g	1000	904.918	904.955	904.927	904.504
Scenario IV (Monod)*, g	1.7724	0.1053	0.01050	-	0.0097

* Analytical solution refers to the results of Simpson and Landman (2007) at t=1.

2.5 Discussion of Results

2.5.1 Non-Reactive Solute Scenarios

The programs TR-FEM and TR-RSE delivered the same results for scenarios I to III for conservative solute conditions. This was expected since both programs use the same transport module of TR-FEM. For the case TRT, two steps of transport are solved for each time step. This improves the results when compared to TR-FEM and TR-RSE because these two programs call the transport module just once every time step for all the non-reactive scenarios.

From Table 2-2 we can observe that the L^2 error norm for scenarios I and II for all the CN and dt combination is almost double the corresponding L^2 error norm for TRT. When results of scenarios I to III are plotted (Figures 2-4, 2-5 and 2-6), there is virtually no visual difference between the three methods. From Table 2-2 we can observe that the numerical simulation approximates the analytical solution better when the temporal step and courant number are reduced. However, this requires more computational effort. For all cases, simulation times were not greater than two minutes. No split operator operation was performed since the reactive term is not used. The mass balance for scenario II showed that the difference between the three numerical methods is not significant to approximate total mass of the plug.

2.5.2 Reactive Solute Scenarios

The programs TR-FEM, TR-RSE and TRT were tested using the four scenarios depicted in Table 2-1. Results in Table 2-3 show that for the same temporal step, TRT approximates the analytical solution better than TR-FEM or TR-RSE (lower L^2 error norm). TR-FEM and even TR-RSE can reach a similar level of accuracy than TRT when Δt is reduced, but at computational cost. For all scenarios, TR-RSE had the lowest Nash–Sutcliffe model efficiency coefficient, even when compared to TR-FEM in the same temporal step due to the TTE.

Scenario I had the best global approximation for TRT, TR-FEM and TR-RSE. When compared visually, the difference among them is minimal (Figure 2-8). The major difference among them can be observed between time 60 and 78 seconds, where a fast change in the slope occurs. This is also supported with the results shown in Table 2-3.

Scenario II better illustrates the difference between the models for approximating the analytical solution. Again, the worst approximation is given when a fast change in the slope occurs, which corresponds to the peak in this scenario. A zoomed section of it (Figure 2-9) shows that TRT and TR-FEM have close levels of approximation to the analytical solution, but TR-RSE slightly underestimates them. The higher value of the L^2 error norm (9.55 for TR-RSE) was obtained in scenario II.

Scenario III may be the one that mimics what could happen under unsteady state conditions because input concentration is changing with time. Here, TRT continues to be the best SO option followed by TR-FEM for all the time steps tested (see Table 2-3 and Figure 2-10). The split TR-RSE split operator method had the worst performance of all. During the inflection points of the graph in Figure 2-10, TR-RSE was the method that most underestimated the solution when compared to the analytical, TRT and TR-FEM

solutions. This agrees with the results shown in Table 2-3 since TR-RSE had the highest L^2 error norm.

Simulation results of the fourth scenario (Monod kinetics) are important because this allows for testing the TRT OS method with conditions other than the simple first order decay kinetics. This scenario also helped to prove that the TRT SO method implemented here is capable of reproducing the results of other works, such as those presented by Simpson and Landman (2007). Simulation results shown in Figure 2-11 overlap the results reported by Simpson and Landman (2007) for the same scenario, showing that the TR-RSE SO method underestimated the solution to Monod kinetics when compared to the TRT method. No formal error analysis was made since no analytical solution was found to have a set of values of reference for Monod kinetics; however, when the solution reported by Simpson and Landman (2007) is used as “analytical solution”, then the global Nash-Sutcliffe coefficient is not very different for both TRT and TR-RSE models (0.99 and 0.98 in scenario IV, Table 2-1). Nevertheless, when the Nash-Sutcliffe coefficient is calculated locally at the peak, then there is a significant difference between the TRT and TR-RSE methods (0.98 and 0.70 for TRT and TR-RSE respectively). The same pattern is observed when the mass balance is performed for scenario IV, where TRT approximated better the solution presented by Simpson and Landman (2007) compared to the TR-RSE method.

2.6 Conclusions

A flexible alternating split operator method was evaluated under simple first order decay and Monod kinetics to solve the 1-D ADR. The flexibility of this program enables the user to enter the equations the program needs to run (in order to numerically solve the reactive term of the ADR for single or multiple species) via a flexible user defined

XML input file. This approach has been applied before by James (2009) in wetlands using a 2-Dimensional finite elements method. TRT has been built in 1-Dimension to be coupled to VFSSMOD (Muñoz-Carpena et al., 1999), which is a 1-Dimensional finite elements method, to solve the transport and reaction of pollutants in surface runoff through vegetative filter strips.

Testing of the TRT alternating SO method with analytical solutions is important to validate the program for future applications. TRT proved to better approximate ADR when compared to TR-FEM and TR-RSE methods for the same time step, For all the scenarios tested either conservative or reactive, the TRT method reported the lower L^2 error norm.

Simulation results also corroborate the results reported by Simpson and Landman (2007) about temporal truncation error removal for alternating SO methods when the temporal step dt is sufficiently small. Underestimation of the analytical solution was more noticeable when a standard TR method was used due to the splitting operation. The TRT alternating showed an important improvement in the efficiency of the solution for complex kinetics, as shown in the Monod example, compared to the tradition TR SO approach (Nash-Sutcliffe coefficients of 0.98 and 0.70, respectively).

The TRT SO program will provide VFSSMOD with the flexibility it needs to simulate the dynamics of pollutants in runoff through VFS, since relationships between pollutant, water, soil and vegetation could conceptually be considered and simulated.

CHAPTER 3
LABORATORY-SCALE TESTING OF A FLEXIBLE MODEL FOR SIMULATING
POLLUTANT TRANSPORT IN DYNAMIC RUNOFF THROUGH VEGETATIVE FILTER
STRIPS

3.1 Introduction

The complexity to solve non-steady state conditions of runoff in VFS has motivated the use of empirical approaches to calculate the pollutant removal efficiency, which generally is based in a few parameters such as filter length and slope. The Soil and Water Assessment Tool (SWAT) filter strip trapping efficiency for sediment, nutrients and pesticides is only a function of the width of the filter strips (Neitsch et al., 2002). Liu et al., (2008) for instance, performed an statistical analysis of various data bases on vegetated buffers and sediment trapping efficacy fitting the data with logarithmic regression models with respect to filter length and slope. The respective r^2 were low, 0.34 and 0.23.

Muñoz-Carpena et al (1993a; 1999) developed a field scale, mechanistic computer model called VFSSMOD-W to simulate hydrology and sediment transport through vegetative filter strips on a storm-by-storm basis. VFSSMOD contains specific submodels to calculate overland flow, infiltration and filtration of suspended sediments. Rudra et al., (2002) implemented an empirical phosphorus component to be used with VFSSMOD-W to estimate the phosphorus yield. However, the removal efficiency of phosphorous is based on two simple concepts: the sediment removal efficiency and an empirical relationship called phosphorous enrichment ratio, which is based on the median particle size of sediment entering to the VFS. Abu-Zreig (2001) also investigated principal factors that affect trapping performance of VFS using VFSSMOD-W. In 2009, VFSSMOD-

W incorporated a water quality module to simulate the removal of pesticides in VFS based on the empirical model developed by Sabbagh (2009).

Due to the strong physical and numerical background of VFSSMOD for simulating transport of water and sediments in VFS, and the effectiveness of the new empirical pesticide module, the US Environmental Protection Agency has included VFSSMOD-W as a recommended model to support the quantification of pesticide reduction in buffer strips as part of a program to maintain watershed health and for the development of control practices (EPA, 2010).

A flexible module to calculate the transport of pollutants in surface water under steady state conditions was developed and analytically tested in Chapter 2. This module needs that an external program that supplies dynamic hydrological data such as runoff water depth, flow velocity, rainfall and infiltration at each node of the domain during the simulation. The coupling of the new transport component with VFSSMOD-W offers the user the possibility to define the processes, equations, parameters, etc that drive the dynamic behavior, and potential reduction of a pollutant in runoff through a VFS. This means that the user can explore a wide variety of conceptual approaches for contaminant transport, from simple empirical to physically-based.

In this work we present the coupling the dynamic hydrological and pollutant transport components (VFSSMOD-W and TRT). The resulting new version of VFSSMOD-W is tested with experimental laboratory data of Yu (2010). Simulation of the experimental data is based on the conceptual model based on the rainfall induced chemical transport theory (Gao et al., 2004).

3.2 Model Development

In this section, VFSSMOD-W and TRT program are presented, followed by the modifications made to VFSSMOD-W for the coupling, including the new input file structure for running the generic flexible water quality module.

3.2.1 Hydrology and Sediment Transport Model (VFSSMOD-W)

The strength of VFSSMOD relies in its numerical calculation of water and sediment balances through a field scale, mechanistic, storm-based procedure designed to route the incoming hydrograph and sedimentograph from an adjacent field through a vegetative filter strip (VFS) and to calculate the outflow, infiltration and sediment trapping efficiencies. The model couples a hydrology submodel to describe overland flow with a sediment filtration submodel based on the one developed at the University of Kentucky (Muñoz-Carpena et al., 1999). Figure 3-1 shows the processes of runoff routing, sediment deposition and infiltration in VFS in the way VFSSMOD-W handles them numerically.

The program relies in four numerical modules: Overland flow, Infiltration, Sedimentation and Water Quality. Communication among these modules is depicted in Figure 3-2.

The surface hydrology submodel used by VFSSMOD-W (Muñoz-Carpena, 1993; Muñoz-Carpena et al., 1993a; Muñoz-Carpena et al., 1999) uses a non-standard Petrov–Galerkin quadratic finite element (FE) overland flow submodel (Muñoz-Carpena et al., 1993a) based on the kinematic wave approximation (Lighthill and Whitham, 1955) of the Saint-Venant overland flow equations.

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = p - f \quad (3-1)$$

$$q = \alpha h^m = \frac{\sqrt{S_0}}{n} h^{5/3} \quad (3-2)$$

where x is flow direction axis (m), t is time scale (s), $h(x,t)$ is vertical flow depth (m), $p(t)$ is rainfall intensity (m/s), $f(t)$ is infiltration rate (m/s), S_0 is bed slope (m/m) at each node of the system, α and m are uniform flow coefficients for coupling Eq. (3-2) (Manning's), and n is Manning's roughness coefficient. VFSSMOD can handle natural, unsteady rainfall conditions in the same rainstorm event. The initial and boundary conditions used are:

$$h=0; \quad 0 \leq x \leq L; \quad t=0$$

$$h=h_0; \quad x=0; \quad t>0$$

$$p=p(t); \quad 0 \leq x \leq L \quad t>0$$

$$f=f(t); \quad 0 \leq x \leq L \quad t>0$$

where h_0 can be 0, a constant or a time dependent function (field incoming hydrograph).

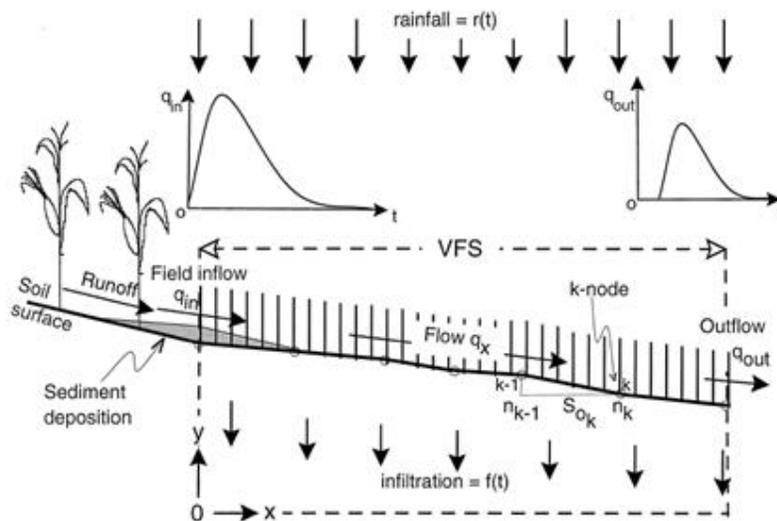


Figure 3-1. Processes and domain discretization for the Finite Element overland flow submodel of VFSSMOD-W (Muñoz-Carpena et al., 1999).

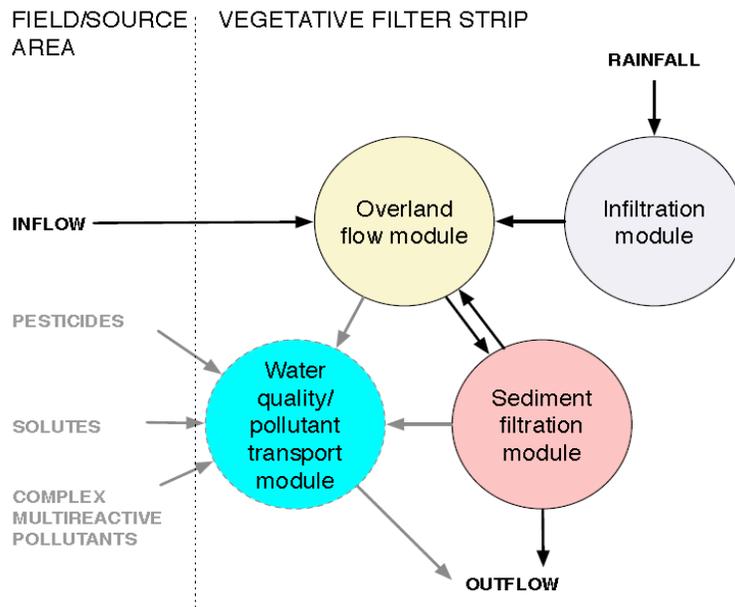


Figure 3-2. Schematic representation of the connection of overland flow, infiltration, particle filtration and pollutant transport modules in VFSSMOD-W. Arrows and text in grey indicate that the pollutant transport module can be turned on when running VFSSMOD-W if needed

The use of a Petrov-Galerkin upwinding formulation to solve equations (3-1) and (3-2) reduces kinematic shock induced the amplitude and frequency of oscillations with respect to the standard Bubnov-Galerkin method (Muñoz-Carpena et al., 1993b), thus improving the model stability. The estimation of the infiltrated water is based on an extended version of the Green-Ampt equation for unsteady rainfall (Chu, 1978; Skaggs and Khaheel, 1982; Muñoz-Carpena et al., 1999).

The time step for the simulation is selected by the kinematic wave model to satisfy convergence and computational criteria of the FEM based on model inputs (Muñoz-Carpena et al., 1993a). The model inputs are specified on a storm basis. Model outputs include detailed hydrographs and pollutographs, mass balance tables for water and sediments and summaries of variables and parameters used in the simulation.

In order to describe the numerical and physical characteristics of the VFS, incoming hydrograph, sedimentograph, pollutograph and rain, VFSSMOD-W needs up to 7 files (if the water quality module is used), but can work only 6 input files. At the end of the simulation, up to six output files (five if not running the water quality module) with detailed data and summarized tables are produced. Table 3-1 shows a description of the input and output files used and generated by VFSSMOD-W.

No details on the sediment transport module of VFSSMOD-W are presented because testing here only includes a soluble tracer (bromide case). For more details about the sediment transport module see Muñoz-Carpena et al.(1999) and Muñoz-Carpena and Parsons (2010).

Table 3-1. Description of the input and output file extensions used in VFSSMOD-W

Input files		Output files	
Extension	Description	Extension	Description
igr	Buffer properties for the sediment filtration submodel	og1	Detailed time series describing the sediment transport and deposition within the buffer.
ikw	Parameters for the overland flow solution	og2	detailed information on the singular points (Muñoz-Carpena and Parsons, 2005).
irn	Storm hyetograph	ohy	Detailed outputs on the inflow and outflow hydrographs.
iro	Storm hydrograph from the source area.	osm	Detailed summaries of the water and sediment balance, final geometry of the filter
isd	Sediment properties for the sediment filtration submodel	osp	Overall summary of filter performance with comparisons between the source area and filter
iso	Soil properties for the infiltration submodel	owq	Details describing the water quality transport and removal efficiency
iwq	Pollutant properties for the Water Quality submodel		

3.2.2 Effect of Pollutant Dilution by Rain

In this section a water balance is proposed to include the dilution of a runoff pollutant that is transported through VFS due to the effect of rainfall. This consideration is being developed to be included in the TRT module before coupling it to VFSSMOD-W

The one dimensional water balance in surface runoff is given equation (3-1), which is given in the kinematic wave equation:

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = p - f$$

where x is flow direction axis (m), t is time scale (s), $h(x,t)$ is vertical flow depth (m), $p(t)$ is rainfall intensity (m/s), $f(t)$ is infiltration rate (m/s) and $q(x,t)$ is discharge (m^2/s).

The concentration of a solute chemical, based on the overland flow mass balance, is given by:

$$\frac{\partial hC}{\partial t} + \frac{\partial qC}{\partial x} = -fC - khC + \frac{\partial}{\partial x} \left(Dh \frac{\partial C}{\partial x} \right) \quad (3-3)$$

where C is the chemical solute concentration (g/m^3) and k is the first order decay coefficient (s^{-1}). and D is the hydrodynamic dispersion (m^2/s).

Developing the partial differential equations on (2-3):

$$h \frac{\partial C}{\partial t} + C \frac{\partial h}{\partial t} + q \frac{\partial C}{\partial x} + C \frac{\partial q}{\partial x} = -fC - khC + \frac{\partial}{\partial x} \left(Dh \frac{\partial C}{\partial x} \right) \quad (3-4)$$

Rearranging common terms in Eq. (3-4)

$$h \frac{\partial C}{\partial t} + q \frac{\partial C}{\partial x} + C \left(\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} \right) = -fC - khC + \frac{\partial}{\partial x} \left(Dh \frac{\partial C}{\partial x} \right) \quad (3-5)$$

Substituting the term $\left(\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} \right)$ based on equation (3-1) on (3-5)

$$h \frac{\partial C}{\partial t} + q \frac{\partial C}{\partial x} + C(p - f) = -fC - khC + \frac{\partial}{\partial x} \left(Dh \frac{\partial C}{\partial x} \right) \quad (3-6)$$

$$h \frac{\partial C}{\partial t} + q \frac{\partial C}{\partial x} = -pC - khC + \frac{\partial}{\partial x} \left(Dh \frac{\partial C}{\partial x} \right) \quad (3-7)$$

Since by continuity equation $q=v \cdot h$, dividing (3-7) by h and re-arranging terms:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - C \left(\frac{p}{h} + k \right) \quad (3-8)$$

Currently, the program TRT has the capability to run a fully coupled finite element method for solving the ADR with a first order decay coefficient (k_1). A global constant $K=p/h+k_1$ can be introduced in equation (3-8) to simplify it and to have the same form than the one used in TRT. However, if a non-reactive compound is used such as a tracer, then $k=0$, reducing equation (3-8) to:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - \frac{p}{h} C \quad (3-9)$$

The term p/h in equations (3-8) and (3-9) accounts for the effect of dilution by rain in overland flow. It is important to point out that the effect of infiltration is included in the water depth in Equations (3-8) and (3-9), although the infiltration ratio does not appear on those equations.

The TRT program (see Chapter 2 for more details) was modified to add the reactive term $K=p/h+k_1$ to account for dilution by rain and a first order decay rate. The advantage of this is that k can be zero, representing a non-reactive compound but keeping the effect of dilution by rain. For the case where no rainfall is present, the p/h is zero and the pollutant might be only affected by the first order decay constant when no infiltration occurs, otherwise infiltration need to be included. For computational efficiency, this term (K) was added to the base finite element transport component,

outside the flexible reactive component (RSE), since dilution by rain will always be present when rainfall occurs.

3.2.3 Chemical Transport Module (TRT)

As described in previous chapter, the TRT program solves the Advection-Dispersion-Reaction Equation (ADR) using a split operator scheme. The transport part of the ADR (Eq. 3-1) is solved using a standard Bubnov-Galerkin cubic/quadratic Finite Element Method for solving the spatial derivatives and a time-weighting (Crank-Nicholson finite difference) method for the temporal derivative. The user defined reactive component solves a system of ordinary differential equations using the fourth order Runge-Kutta method. Each equation represents the change of some specific pollutant in time. Pollutants can be considered as mobile or stable, depending if they move with runoff (i.e. soluble compounds) or stay in the same place during the simulation (i.e. pollutant soil porewater concentration, adsorbed pollutant to soil and vegetation, etc). Mobile and stable elements are related using ordinary differential equations to obtain a mass balance for each time step. The program performs a Transport-Reaction-Transport split operator scheme at each time step. This means that the pollutant is transported using half of the time step, then is reacted for the full time step, and then transported for the remaining time step. Results presented in previous chapter during analytical testing of the TRT module showed the accuracy of this is slightly better when compared to the fully coupled finite element method (TR_FEM) for simple first order decay reaction and Monod kinetics (see section 2.4.1 and 2.4.2).

The TRT program (stand-alone version for steady state conditions) needs three input sets to run: one that includes the transport and numerical parameters to be used by the transport module, and two for describing the user-defined properties and

parameters of the mobile and stable compounds and the equations to be used, written in XML format. The input parameters and structure for running TRT module can be seen in Tables A-1, A-2 and A-5.

The main limiting factor when running the stand alone TRT program is that it runs with constant runoff depth and velocity through the domain and does not consider the effect of dilution by rain. Dynamic conditions are very important when dealing with field scale or experimental data because they usually change with time, as infiltration does during a rainfall event.

3.2.4 Model Linkage

When TRT is used, the pollutant concentration is calculated at each time step, and then passed to the reactive module to complete the change of concentration in time. The time and spatial steps and the flow velocity are input to the model as constant during the simulation. VFSSMOD-W can produce the hydrologic and numerical data that TRT needs at each time step through the domain (filter length) for dynamic flow conditions. The procedure to link these two programs includes: 1) to transfer the spatial and temporal steps and other numerical parameters from VFS MOD-W to TRT, 2) to modify the ADR used in TRT to include the effect of dilution and code it in the transport module of TRT, 3) to call TRT once the hydrodynamic flow parameters are calculated in VFSSMOD-W.

The TRT module (see section 2.2.3) was designed to be coupled to VFSSMOD-W to simulate the dynamics of pollutants in runoff through VFS. Since both programs share the finite element method, the transport module of TRT and VFSSMOD-W have various subroutines in common, especially those related to solving the matrices

generated by the finite element method. This allowed for efficient coding with standard structure for both components.

The TRT split operator program uses the next numerical parameters: Spatially discretized length in the X direction ΔX , time step ΔT , Number of time steps for the simulation N_{DT} , time weighting method for the temporal derivative (0.5 for Crank-Nicholson) θ , order of the integration rule NL over each element and the number of nodal points over each element $NPOL$. These parameters are transferred directly from VFSSMOD-W to TRT during the simulation.

The hydrological parameters used by the TRT program are: the length L of the domain in the X direction, the longitudinal dispersivity $DISL$ (α_L in Eq. 2-2), the molecular diffusion coefficient $DISM$ and the first order decay reaction coefficient K_1 . For this set of parameter, only the length L has its equivalent with the buffer length VL in VFSSMOD. The rest of the parameters are new for VFSSMOD-W so they need to be input as new parameters.

None of the chemical parameters is declared or used in VFSSMOD-W. So all the water quality parameters used in the TRT program have to be input as new parameters in VFSSMOD-W. However, the structure of the input files need to be adapted to have fully compatibility with the current file organization in VFSSMOD-W.

The modifications to the structure of the *.iwq water quality input file is detailed in Appendix A. Based on these modification, there possible options are handled in VFSSMOD-W to simulate the transport of pollutants: 1) Transport of pesticides based on an empirical equation developed by Sabbagh et al. (2009), 2) solely transport of a solute in runoff through VFS considering the effects of dilution by rain and infiltration

and, 3) The multi-component flexible approached based on the TRT module. A schematic representation of VFSSMOD-W with the new water quality module is shown in Figure 3.3.

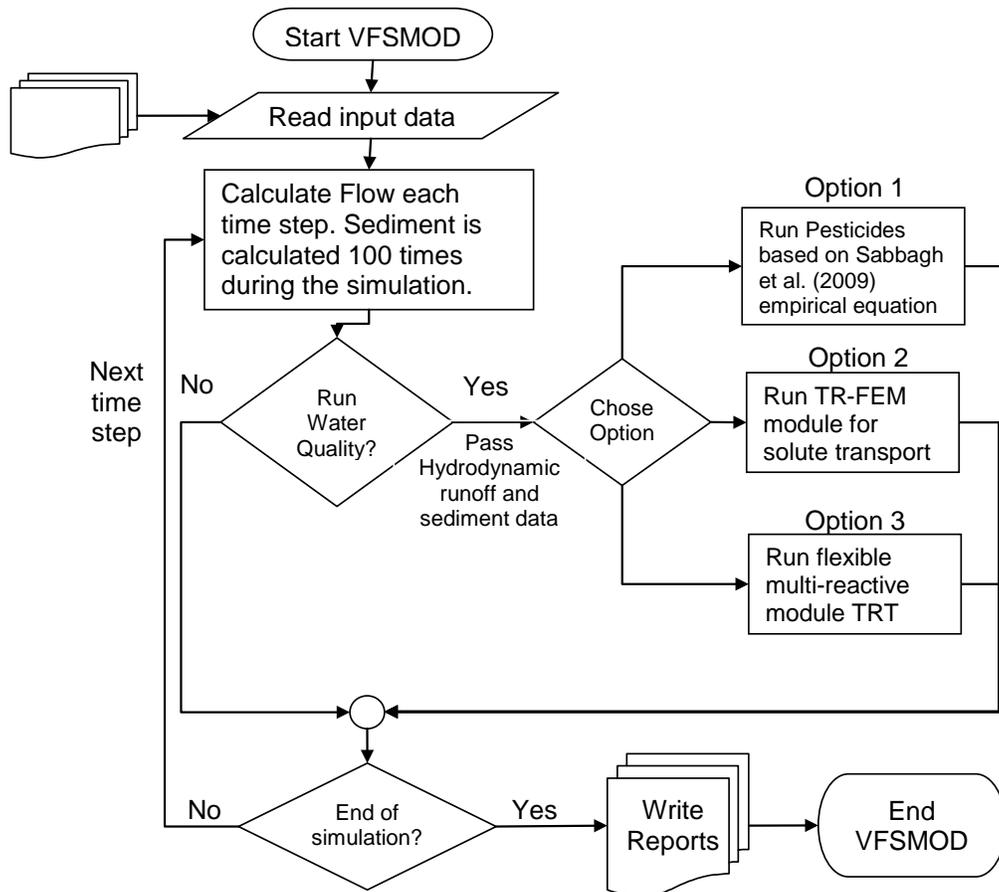


Figure 3-3. Schematic representation of linkage between VFSSMOD-W and the water quality module.

3.3 Model Testing

In order to test the new flexible water quality module of VFSSMOD-W, data from Yu et al. (2010) experiment is used. The laboratory experiment was conducted to investigate the processes involved in the transport of nanoparticles in surface runoff. A laboratory scale experiment was designed to study runoff with five basic considerations:

- 1) a sand bed box with no vegetation on top receives artificial rainfall and lateral runoff,

2) a plug of pollutant is injected with the lateral runoff, 3) infiltrated water is collected from a drainage system, 4) runoff is collected at the end of the box and 5) samples of runoff and infiltrated water are collected and analyzed. The absence of vegetation and homogenous soil allows for a controlled experiment with a reduced number of variables. A description of the experiment and the conceptual model used to explain the data is depicted in the next sections.

3.3.1 Experimental Setup

Yu et al. (2010) designed an experiment to investigate the surface transport of nanoparticles (kaolinite) in runoff compared to that of a conservative tracer. The experiment was conducted in the Water Resources Laboratory of the Agricultural and Biological Engineering Department at the University of Florida. A schematic representation of the experiment is shown in Figure 3-4.

In Yu's experiment a metal box (1.53 m long, 0.402 m wide and 0.10 m deep) is built and divided in four equidistant compartments of 0.38 m separated by metal divider of height of 0.05 m are used to make the compartments. Each compartment was fully filled with 12 kg of sand with a media size of 0.55 mm. Bulk density of sand reported by Yu (2010) was 1.538 g/cm^3 and the estimated saturated hydraulic conductivity was $1.06 \times 10^{-5} \text{ m/s}$. A vertical drainage system collection system was added to the soil box by making a 1 inch screwed sinkhole in the bottom of each compartment for a total of four. The drainage is centered to the downslope end of each compartment. A 500 mesh screen was used in each sinkhole to cover them so only water can be filtrated. A funnel with a 1.27 cm diameter hose was connected through each drainage sinkholehole in order to collect the infiltrated water into 22.7 liter cylindrical bucket buckets. A runoff collector was installed at the end of the box and connected similarly to the drainage

system to a 22.7 liter cylindrical bucket. Water depth in each bucket was measured using a dielectric capacitance probe (ECH₂O 20 cm probe, Decagon, Pullman, WA) every thirty seconds and then correlated to volume. Data was stored in a automatic data logger (CR40, Campbell Sci, Pullmand, WA).

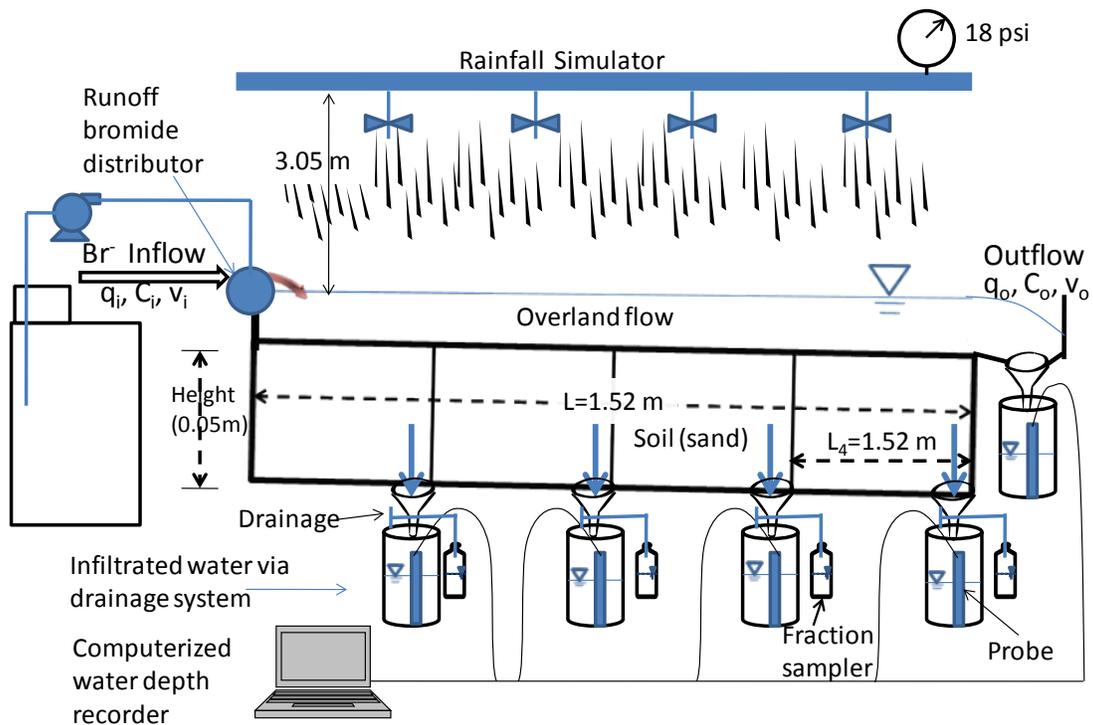


Figure 3-4. Schematic representation of the laboratory experiment used by Yu et al. (2010).

Rain was produced using a rainfall simulator with a stainless steel Tee Jet 1/2 HH SS 50 WSQ nozzle (Spraying Systems Co.,Wheaton,IL) located approximately 3 m above the box. Experiments were conducted under the pressure of 1.24 bar (18 psi) which generated rainfall intensity of 64 mm/hour with uniformity greater than 90% over the box. The rainfall intensity was monitored and measured by 6 standard garden rain gauges and one electronic tipping bucket rain gauge (Texas Electronics Inc.,Dallas, Texas) connected to the data logger.

The pollutant inflow rate was set to 0.3 l/min with a peristaltic pump (Master Flex L/S digital standard drive pump, Cole-Parmer Instrument Company, Vernon Hills, Illinois). Precision pump tubing transports the inflow to a spreader for uniform water and solute distribution over upslope end of the box (Figure 3-4).

In order to reach steady state conditions for the experiment, the sand was saturated by the simulated rain for two hours prior to the experiment in order to assure saturation conditions and no bromide presence in the media. After saturation was reached, a 103 mg/l pulse of bromide is release for 30 minutes. When the pulse of bromide is over, clean water is continuously injected at 0.3 l/min until the end of the simulation in order to do not affect the water balance. Artificial rainfall is constant during the entire experiment as well. The output runoff and infiltrated pollutant is measured for 50 more minutes to complete a total time of 80 minutes, starting at the time the pollutant is released in runoff. Water samples were taken during the 80 minutes of the experiment and then analyzed using an ion chromatograph (Dionex ICS90) to determine bromide concentrations in water samples.

3.3.2 Conceptual Model

One of the most critical processes for simulating pollutant transport in runoff is the movement of pollutants from soil to runoff. Extensive research has been conducted over the past thirty years in an attempt to explain the mechanisms involved in this process. The most widely applied theories are the film theory (Wallach et al., 1989; Wallach and Vangenuchten, 1990; Wallach, 1991), the chemical mixing depth concept and its variations (Ahuja, 1982; Steenhuis et al., 1994; Zhang et al., 1997) and the raindrop solute transfer theory (Gao et al., 2004). In the film theory, the pollutant is transported by molecular diffusion to a thin layer or film of water that lies between soil and runoff.

The chemical mixing concept theorizes that the pollutant is mixed instantaneously in a zone below the soil, which includes water from rain, runoff and infiltrated water. This mixing zone can be considered to be either uniform and complete, uniform but incomplete, or non-uniform and incomplete (Zhang et al., 1997). Wallach and van Genuchten (1990) indicated based on their results that direct mixing between runoff water and the soil solution is responsible for chemical transfer only during the early stages of the runoff process, but later the convective mass transfer becomes the main transport mechanism. Walton et al. (2000) proposed that the release of a pollutant from soil to runoff should consider the soil moisture condition previous to the rainfall, as opposed to under saturated conditions, as assumed in most of the experiments designed to study this transfer. Walton et al. (2000) introduced the concept of the blind-pore factor to account for pollutant that remains in the soil surface once the initial rainfall has infiltrated part of the pollutant from the surface soil, and tested this theory using field site experimental data but concluded that some processes occurring at early times were not adequately described by his model. Finally, Gao et al. (2004) introduces the concept of soil exchange layer, where the pollutant is release from porewater soil stored in an exchange layer near the surface, when raindrops hit the ground. In Gao's study, a combined raindrop-controlled solute transfer and diffusion process was used to explain experimental data under no flow conditions. Gao et al (2004) concluded that other phenomena, such as the pumping mechanism or a different interaction between raindrop-induced solute transfer and diffusion, were required to properly simulate solute transfer from soil to runoff. The pumping mechanism depicted by Gao is similar to interflow depicted by Ahuja (1982). At a larger scale, this pumping mechanisms has

also been studied by Packman et al. (2000) to describe the advective flow of pollutants induced in a sand bed by stream flow over bedforms. Figure 3-5 shows the schematic representation of the bromide exchange between runoff and porewater using the exchange layer proposed by Gao under dynamic flow conditions.

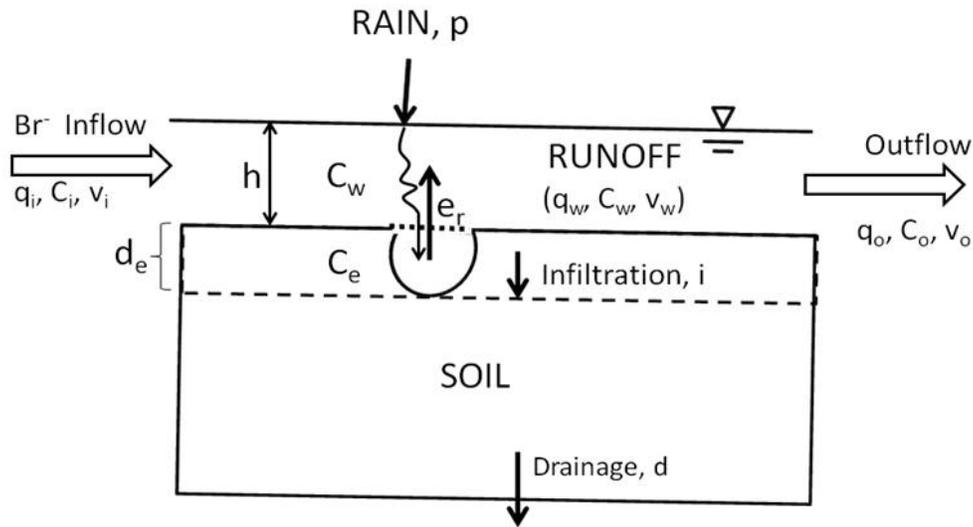


Figure 3-5. Conceptual schematic representation of physical and chemical transport processes in runoff Bromide in Yu's (2009, unpublished) experiment.

In Figure 3-5, C_w and C_e represents the concentration of bromide in surface runoff and porewater respectively, i represents the infiltration rate, and e_r is the rate of soil water that is ejected into the runoff.

The balance of Bromide in surface runoff used in Yu et al. (2010) experiment can be described using the next ordinary differential equation based on Figure 3-5.

$$\frac{dC_w}{dt} = -\frac{e_r}{h}(C_e - C_w) \quad (3-10)$$

where h represents the runoff depth.

From the perspective of change in concentration in porewater, we have

$$\frac{dC_e}{dt} = iC_w - iC_e + e_r(C_w - C_e) \quad (3-11)$$

Equation (3-11) can be simplified as follow

$$\frac{dC_e}{dt} = \frac{i + e_r}{d_e} (C_w - C_e) \quad (3-12)$$

Where d_e represents the effective layer depth.

A factor α is introduced by Gao et al. (2004) that accounts for incomplete mixing of the pollutant in runoff with rain before infiltration. In this study α accounts for the incomplete mixing of pollutant in soil. This is because the depth of flow in this experiment is much smaller than that used under the ponding conditions of Gao et al. (2004). The mixing factor α can have a valid range $0 \leq \alpha \leq 1$. The system of ordinary differential equations that controls the movement of a non reactive pollutant such as bromide is given by equations (3-10) and (3-12). When the mixing factor α is introduced, the system of equations is defined by:

$$\left\{ \begin{array}{l} \frac{dC_w}{dt} = -\frac{e_r}{h} (\alpha C_e - C_w) \\ \frac{dC_e}{dt} = \frac{i + e_r}{d_e} (C_w - \alpha C_e) \end{array} \right. \quad (3-13)$$

Since Yu et al. (2010) laboratory scale experiment included rain, the rain-drop controlled solute transfer theory proposed by Gao (2004) was chosen to predict Yu's experimental data together with a simple uptake/release model as the one depicted in Figure 2-3, which is driven by the system of equations (2-25) and (2-26), where the constants K_u and K_r represent the exchange rate of Bromide between the surface water column (runoff) and the bromide in porewater. These empirical constants are an empirical simplification of the different physical mechanisms proposed when Bromide is exchanged between surface water and porewater, such as diffusion, pumping (Packman et al., 2000), raindrop effect (Gao et al., 2004), etc. The variables C_w and C_s

(Equations 2-25 and 2-26) represents the concentration of bromide in surface runoff and porewater respectively.

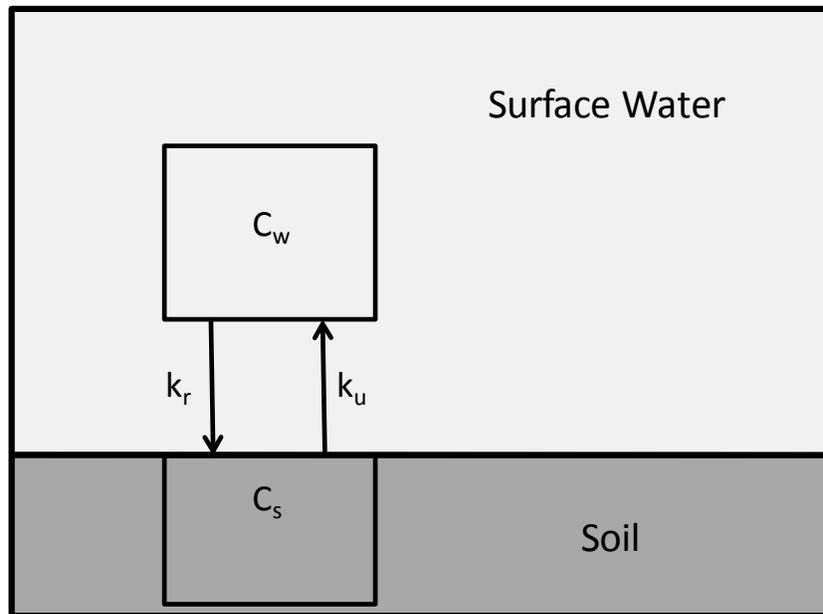


Figure 2-3. Basic conceptual model for uptake/release dynamics of phosphorus between the soluble phosphorus in water column and settled phosphorus on soil. Source: Adapted from James (2008b) as shown in Chapter 1.

3.3.3 Input Parameters for the Water Quality Module

Based on the system of equations formed by equations (2-13) and (2-14), two input sets need to be created (contained in the program *.iwq and the XML water quality input files).

We first have to define the elements that are represented in the system of equations. From the left hand side of equations (3-13) and (3-14) we observe one mobile component C_w (bromide in runoff) and one stable component C_e (bromide in porewater). From the right hand side of these equations, besides C_w and C_e , there are five parameters: e_r , i , h , d_e and α . The water quality input file (sampleBr.iwq) containing all these elements and its corresponding values are presented in Table A-8 in Appendix A. The system of reaction equations and the definition of the variables and parameter to

be used during the simulation are contained in the user-defined XML input file (“YuGao.xml” see Table A-8, Appendix A). A detailed description of each of the VFSSMOD-W input files used for running this simulation is also presented in Appendix A. For the empirical approach using k_u and k_r , the XML input file is shown in Table A-2 in Appendix A. Table 3-2 shows a summary with the most important parameters used for testing the empirical and mechanistic approaches.

Table 3-2. List of parameters used in the physically based and empirical conceptual models for bromide transport

Parameter	Description, units	Value used in simulations	Recommended value*
e_r	Raindrop induced water transfer rate, m/s	2.5×10^{-7}	$1.5 \times 10^{-6} - 8.4 \times 10^{-6}$
d_e	Exchange layer depth, m	0.05	0 - 0.1
α	Concentration mixing factor, dimensionless	0.1475	0-1
K_u	Pollutant release rate, s^{-1}	0.0093	-
K_r	Pollutant uptake rate, s^{-1}	0.2	-

* Gao et al. (2004).

3.3.4 Model Testing Procedure

Three steps were followed in order to test the flexible water quality module of VFSSMOD-W using the experimental data of Yu et al. (2010). First, measured data of rain, inflow, tracer plug duration, concentration, etcetera of the experiment were properly parametrized to be included in the input files of VFSSMOD-W. Second, since rainfall and runoff inflow did not change in time, an inverse calibration procedure was used to define the values of the infiltration parameters (average suction at the wetting front and saturated hydraulic conductivity) to fit the measured runoff output flow. Water balances of rain, inflow, infiltration and outflow were performed and compared to those obtained during the experiment. Finally, once the water balance was satisfactory, the

water quality module was used to include the release of bromide from soil to runoff based on the system of equations (2-25) and (2-26) for solely transport of bromide, the simple uptake/release empirical approach, and (3-13) and (3-14) for the mechanistic Gao's exchange layer theory.

For the case of the rainfall induced chemical transport (exchange layer) theory, the model was first tested using the recommended values of Table 3-2. However, it was not possible to reproduce the experimental data and various combinations of the conceptual model parameters were used in order to reproduce the experimental data (Figure 3-6). The best fitting was obtained when the parameters reported in Table 3-2 were used (Figure 3-8).

For the case of the empirical uptake/release conceptual model, different values of k_u and k_r were tested in order to obtain the best combination that reduced the error (Figure 3-8). Since these parameters are purely empirical, the values reported in Table 3-2 are valid only valid for those conditions of the experiment.

3.4 Results

3.4.1 Experimental Results

Experimental water balances are summarized in Table 3-3. Values of inflow runoff and rain rate are considered constant during the entire time of the experiment and simulation since they are fully controlled during the experiment (see section 3.3.1). In this table, a mass-balance deficit close to 5% is shown, which is deemed acceptable. The deficit could be related to the soil porewater content at the end of the 80 minutes since only the total water collected in the drainage/runoff collection system (see Figure 3-3) is reported for mass balance. The surface area of the sand box (1.52m x 0.402m) is used to transform units from m^3/s to mm/h.

Table 3-3. Water Balance of Yu et al. (2010) laboratory experimental results.

Parameter/variable	mm/hr	L/min
Inflows		
Runoff inflow	29.03	0.3000
Rainfall	64.17	0.6532
Outflows		
Drainage	37.86	0.3856
Runoff	49.93	0.5085
<i>Subtotal inflows</i>	<i>93.20</i>	<i>0.9532</i>
<i>Subtotal outflow</i>	<i>87.79</i>	<i>0.8941</i>
<i>Mass Balance Error (%)</i>	<i>-6.3</i>	<i>-0.15</i>

The bromide concentration in time for each one of the four compartments of the infiltration system and outflow runoff is presented in Figures (3-6) and (3-7) and the mass balance based on these breakthrough curves is shown in Table 3-3. Time scale is reported from 0 to 80 minutes. Infiltrated (drainage) bromide has different breakthrough curves for each compartment. This was not only because the concentration in time was different along the length of the sand box in surface runoff, but because the average infiltration drainage rate in each of the four compartments was different (0.1071, 0.1193, 0.0754 and 0.0938 L/min).

As stated before, starting time ($t=0$) corresponds to the time when bromide is injected to inflow runoff, and the final time of 80 minutes corresponds to the ending time of data measurement. Thus the previous 120 minutes of rainfall to take the experiment to steady state conditions is not reported. Bromide concentration at inflow is set to constant with a value of 103 g/m^3 for the 30 minutes of duration of the pulse.

A deficit of bromide (12%) is observed for the experimental data (Table 3-4). This deficit can be related to the dissolved phosphorus held in pore water at the end of the simulation. From Table 3-4 we can observe that 35.8% of the incoming mass of bromide

leaves the sand bed as outflow runoff, and 53% of bromide mass leaves the system through the drainage system.

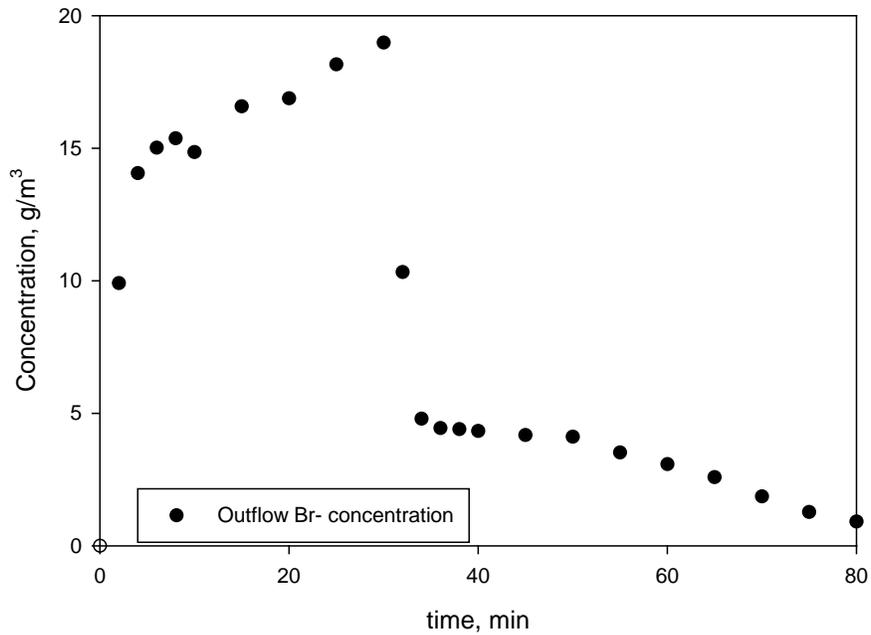


Figure 3-6. Experimental surface outflow runoff bromide concentration as reported by Yu et al. (2010).

Table 3-4. Bromide mass balance of Yu et al. (2010) experimental results.

Parameter/variable	Br ⁻ Mass, g
Inflows	
Runoff inflow	0.927
Outflows	
Drainage 1	0.208
Drainage 2	0.171
Drainage 3	0.074
Drainage 4	0.039
Runoff outflow	0.332
<i>Subtotal inflows</i>	<i>0.927</i>
<i>Subtotal outflow</i>	<i>0.824</i>
<i>Mass balance error</i>	<i>-0.103 (-12%)</i>

3.4.2 Water Balances using VFSSMOD-W

VFSSMOD-W was run without the water quality module and with no sediments from the upland inflow in order to simulate the runoff outflow and infiltration reported in the

experiment. Since infiltration rate was not homogenous in each compartment of the sand box, the inverse calibration module of VFSSMOD-W was used to estimate the optimized calibration values of the vertical saturated hydraulic conductivity VKS, the Green-Ampt's average suction at wetting front SAV, manning coefficient and mean slope of the sand box. The hydrological input parameters used for the water balance simulation are summarized in Table A-9.

With the help of the inverse calibration module of VFSSMOD-W, the difference between the amounts of water at the input (rain, inflow) and output (outflow, infiltration) during the simulation was less than 0.15%. A comparison between the simulated water balances and the experimental data is presented in Table 3-5. It should be noticed the fact that simulated infiltrated (drainage) water is greater than the experimental data. This may be due to the experimental deficit already observed in Table 3-5.

Table 3-5. Water Balance of Yu et al. (2010) experimental results.

Parameter/variable	Experimental data, L/min	Simulated data, L/min
INFLOWS		
Runoff inflow	0.3000	0.3000
Rainfall	0.6532	0.6532
OUTFLOWS		
Drainage	0.3856	0.4432
Runoff	0.5085	0.5085
<i>Subtotal inflows</i>	<i>0.9532</i>	<i>0.9532</i>
<i>Subtotal outflow</i>	<i>0.8941</i>	<i>0.9517</i>
<i>Mass balance error</i>	<i>-6.3%</i>	<i>-0.15%</i>

3.4.3 Bromide Simulations using VFSSMOD-W with the TRT Module

Once the VFSSMOD-W hydrology component was successfully tested, the water quality module TRT was used to simulate the bromide experimental results obtained by

Yu et al. (2010). For the empirical approach, equations 2-25 and 2-26 with $C=103\text{mg/l}$, $k_u=0.22\text{s}^{-1}$ and $k_r=0.0087\text{s}^{-1}$ are used. The corresponding input file is similar to that depicted in Table A-7. For the exchange layer theory, the system of equations defined by Equations (3-13) and (3-14) is used as depicted in Table A-8, and the XML input file is available in Appendix A.

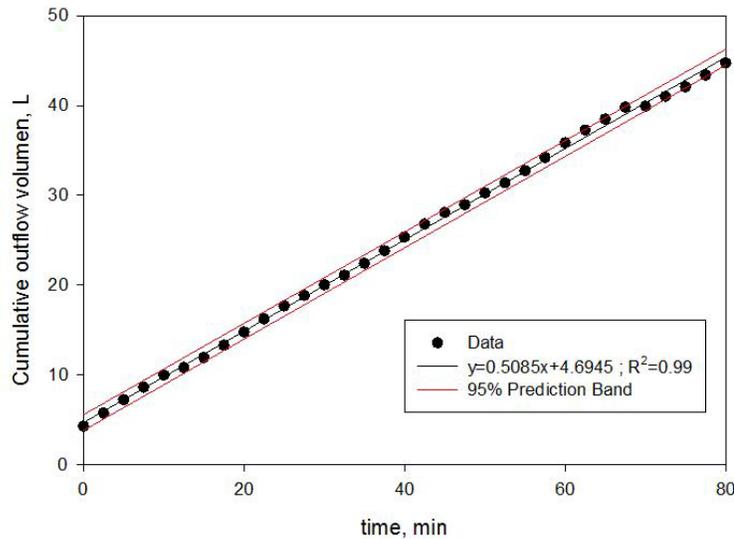


Figure 3-7. Cumulative outflow runoff volume of experimental data. The estimated average outflow rate is 0.5085 L/min.

As stated in section 3.3.4, three scenarios were tested for the transport of bromide in surface runoff: 1) Only transport, 2) Uptake/release empirical approach and 3) Mechanistic exchange layer theory (Gao et al., 2004). Simulation results of each scenario and experimental data are shown in Figure 3-8. The dot-dash line shows the simulation based on solely transport simulation. The dashed line is the better simulation obtained for the exchange layer theory by using the recommended values of Table 3-2 and extending the value of the raindrop induced water transfer slightly out of the lowest recommend value. It is important to point out that recommended values in Table 3-2 are based on static (no dynamic) flow conditions and a greater water depth (Gao et al.,

2004). Finally, for the empirical conceptual model (continuous line), various combinations of the uptake and release rate constants k_u and k_r were used to fit the experimental data by trial and error. The best results were obtained when $k_u=0.22s^{-1}$ and $k_r=0.0087s^{-1}$.

In Figure 3-8 we can also observe that the experiment is driven by two phenomena: A transport of bromide dominated by the hydrodynamic dispersion during the first 30 minutes of the simulation followed by a long tail related to the release of bromide from porewater due to the raindrop effect on the exchange layer and other processes. Mass balances for Figure 3-8 are summarized in Table 3-6.

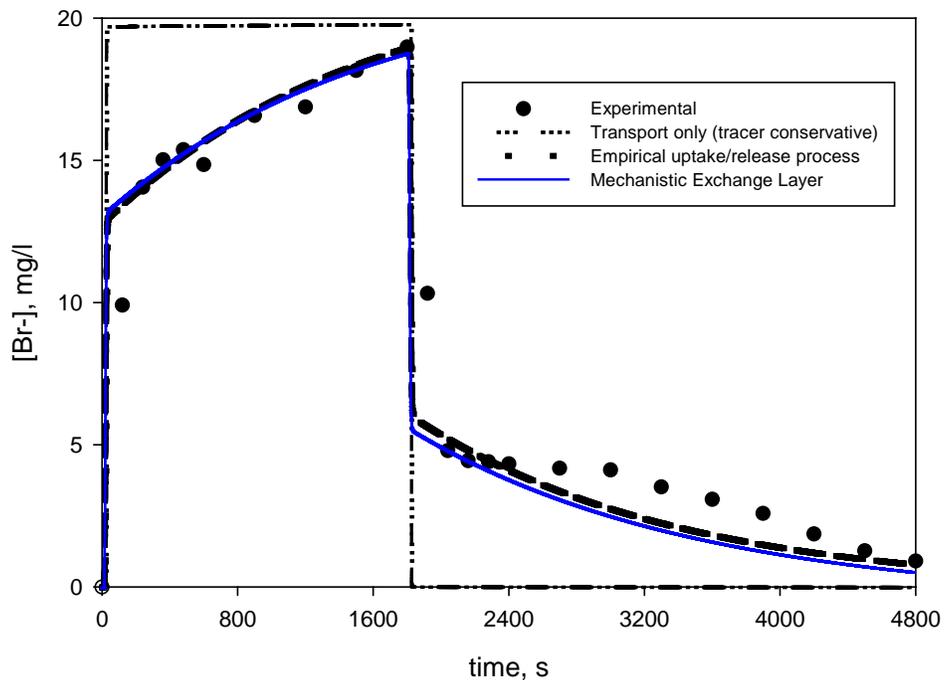


Figure 3-8. Concentration during the simulation of bromide in runoff at the end of the sand box ($x=1.52$ m). Bromide was released as a plug during $0 < \text{time} < 30$ min with a constant concentration of 103 mg/l.

From Table 3-6 we can observe that in terms of total mass of bromide during the 80 minutes of the experiment, the empirical and the mechanistic approach estimated in 96% the total amount of bromide reported with the experimental data (Nash-Sutcliffe

coefficient of 0.94 and 0.95 respectively). The scenario that considers the sole effect of transport of bromide underestimates the experimental mass in 9%. However, these global results of mass balance can mask the fact that the transport only approach overestimate the load and concentration of bromide during the first 1800 seconds of the simulation, which compensated the absence of a tail. In contrast, empirical and mechanistic approaches can reproduce very accurately the first 1800 seconds, and simulate a general trend of the tail.

Table 3-6. Mass balance of bromide in surface runoff for experimental and simulated results.

	Experimental	Simulated		
	(g)	Transport only	Empirical approach	Mechanistic approach
Runoff inflow	0.927	0.927	0.927	0.927
Runoff outflow	0.332	0.3013	0.319	0.318
Predicted error (%)		9.24	3.94	4.24

The big disadvantage when using the empirical approach is that the constants lack of applicability beyond the conditions of this experiment. In contrast, a mechanistic approach is applicable to various conditions and scenarios due to its physically based development.

3.4.4 Sensitivity Analysis of Transport Component

During the simulation of the mechanistic approach, the values of D_L (longitudinal dispersivity), e_r (rate of soil water release due to rainfall effect), d_e (depth of exchange layer), and α (effective mixing effect in runoff) were adjusted to fit experimental data (Figure 2-8). A simple sensitivity analysis was performed by varying these parameters by $\pm 25\%$ and $\pm 50\%$ with respect to the effective base values that best fitted the experimental results as shown in Figure 3-9.

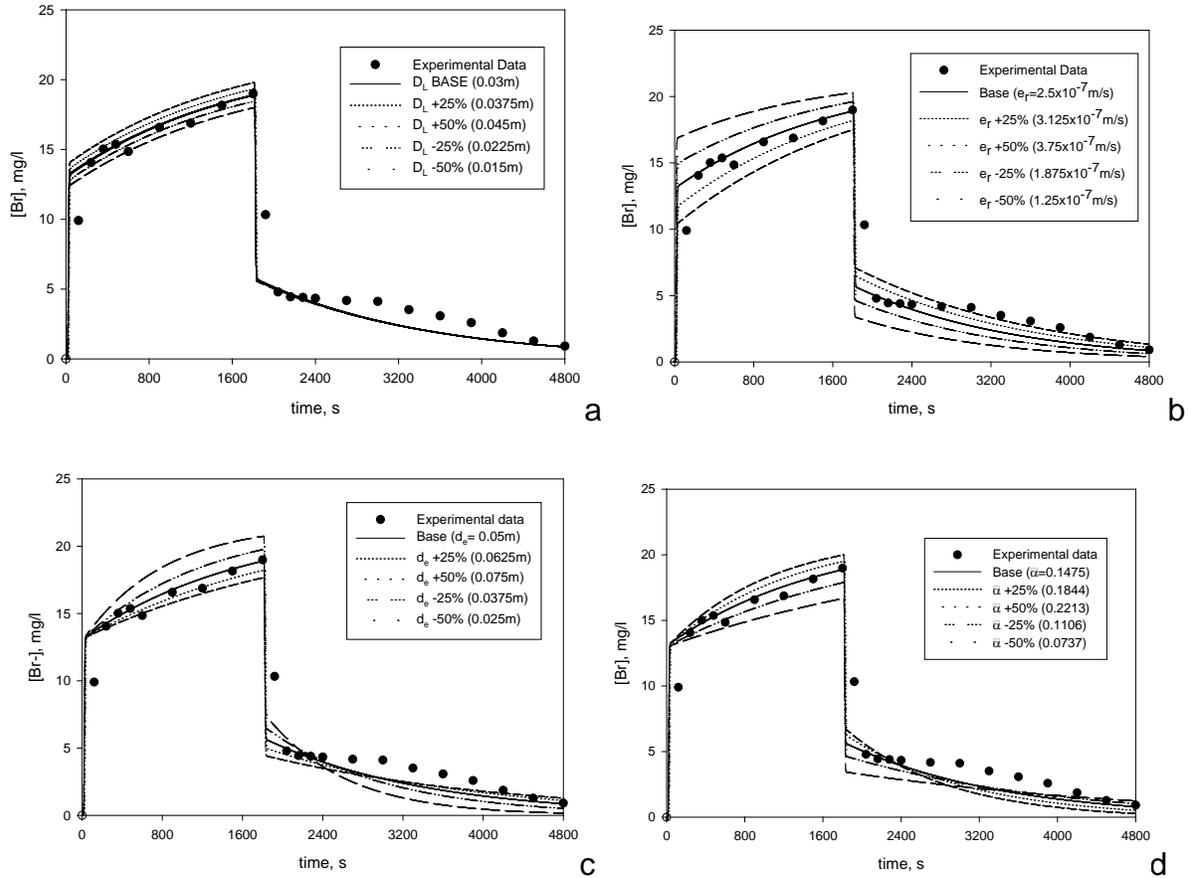


Figure 3-9. Sensitivity analysis of outflow runoff bromide concentration for the variables D_L (a), e_r (b), d_e (c) and α (d), by varying $\pm 25\%$ and $\pm 50\%$ the calibrated values for exchange layer approach.

The Nash-Sutcliffe coefficient was not used during the sensitivity analysis because an overestimation-underestimation compensation occurs between the first 30 minutes of the simulation when advection dominates the transport of bromide, and the next 50 minutes where the release of bromide from the sand bed occurs (see Figure 3-9 b, c and d). A better appreciation of the influence of the variation of the parameters over the outflow concentration during the simulation is represented in Figure 3-9.

The sensitivity to the parameters D_L , e_r , d_e and α for the exchange layer physically based approach with respect to the total mass (area under the curve) and the concentration peak, is shown in Figure 3-10.

Exchange layer theory parameters e_r , d_e and α showed to have small sensitivity to the total mass of bromide (from -4% to 4% in Figure 3-10a) but is more sensitive for peak of concentration of bromide (from -12% to 10% in Figure 3-10b).

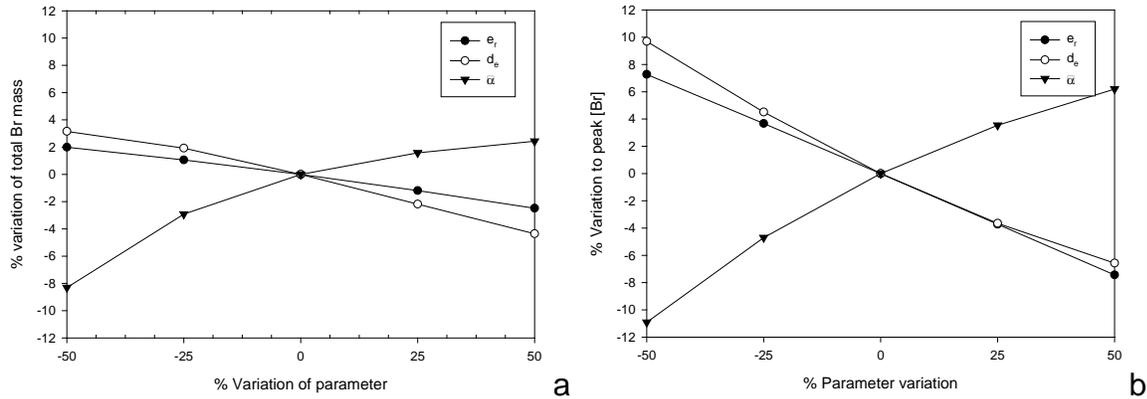


Figure 3-10. Sensitivity response of outflow runoff bromide concentration for the variables D_L , e_r , d_e and α with respect to the total mass (a) and concentration peak (b), by varying $\pm 25\%$ and $\pm 50\%$ the calibrated values for exchange layer approach.

3.5 Conclusions

Experimental water balances were well simulated when using VFSSMOD-W, confirming to be a very reliable model to simulate the outflow runoff in vegetative filter strips (water mass balance error $< 0.15\%$). The inverse calibration module of VFSSMOD-W was helpful to calibrate the model before the simulation of a pulse of bromide in runoff.

Three approaches were used to simulate the experimental results of bromide transport in runoff in a sand bed: one based on the transport of bromide in runoff without other considerations, another based on the physically based rainfall induced chemical transport (exchange layer) theory and the last one using a simplistic empirical approach. For the exchange layer theory, a Nash-Sutcliffe coefficient of 0.95 was obtained when the recommended values of the parameters were modified. This might indicate that the

based rainfall induced chemical transport theory is not enough to explain the experimental results for bromide under dynamic runoff conditions and that other processes such as the diffusion of bromide from porewater to runoff, pumping effect, etc need to be considered to parameterize the conceptual model. It is important to point out that the exchange layer theory was experimentally developed for no flow conditions (Gao et al., 2004). For the second approach, an empirical uptake/release process approximates the experimental data with a Nash-Sutcliffe coefficient of 0.94. However, there is no certainty that the empirical values of the uptake and release constants could work for other conditions different to those used in the experiment.

The new flexible module TRT coupled to VFSSMOD-W opens a new window of possibilities to study the transport and reaction of pollutants in surface runoff through vegetative filter strips. This model can be used either to test current theories for specific pollutants or to explore different physically based processes that could be involved in the transport of runoff pollutants. By using physically based processes instead of empirical relationships, the model can be used for various laboratory and field conditions.

CHAPTER 4
FIELD-SCALE TESTING OF A FLEXIBLE MODEL FOR SIMULATING MINING
TAILINGS PHOSPHORUS TRANSPORT IN RUNOFF USING VFSSMOD-W

4.1 Introduction

Research about vegetative filter strips during the last 20 years has focused on measuring removal efficiencies for different pollutants and establishing mostly empirical relationships to predict the efficiency of a filter based on one or two parameters such as filter length or slope (Neitsch et al., 2002; Liu et al., 2008). Those relationships are usually easy to use, but their accuracy is limited to the set of field or laboratory conditions that were used to obtain the regression equations. Their application to other conditions of soil, type of vegetation, slope, etc is also limited and the efficiency coefficients are generally low. In order to deal with this problem, Muñoz-Carpena and Parsons (1999; 2004) designed a field scale, mechanistic, storm-based model called VFSSMOD-W to handle incoming hydrographs and sedimentographs from an adjacent field through VFS. VFSSMOD-W has been effectively tested with different scenarios (Muñoz-Carpena et al., 1999; Abu-Zreig, 2001; Zhang et al., 2001; Abu-Zreig et al., 2003; Kuo and Muñoz-Carpena, 2009). In 2009, an empirical equation (Sabbagh et al., 2009) was coupled to VFSSMOD-W to estimate the removal of pesticides in VFS.

In previous chapters, a flexible water quality module was added to VFSSMOD-W to simulate a wide number of pollutants based on a user defined system of equations that describe the dynamics of pollutants in surface runoff. This novel approach was tested with a set of experimental data provided by Yu et al. (2010) to simulate the transport of bromide in runoff under laboratory scale experimental conditions. The tool has the potential to simulate field scale scenarios.

The testing of the flexible water quality module of VFSSMOD-W under field scale conditions is presented here. The main objective is to predict the transport of dissolved phosphorus (DP) in runoff from phosphate mining tailing areas typical of central Florida (Polk County) when using vegetative filter strips. Phosphorus dynamics in VFS will follow the processes described by Kuo (2007), who found that pH dependent apatite dissolution from tailing materials can contribute to the loads of dissolved phosphorus. The concentration of particulate phosphorus is not included in this work because of two considerations: 1) It is linearly related only to the fraction of sediments in the outflow (Kuo, 2007; Kuo et al., 2009) and 2) The rainfall event to be simulated contains one of the lowest concentrations of dissolved phosphorus during field experiment, which reduced the sources of particulate phosphorus to be added to the runoff.

If successfully tested, the new water quality module of VFSSMOD-W will give the researchers, decision making personnel, or governmental agencies, a reliable and tested tool to estimate the optimal length of VFS needed to remove a specific pollutant in runoff for different situations and scenarios.

4.2 Experiment Description

Two experimental sites were constructed in 2005 by Kuo (2007) to study the efficiency of VFS for removing phosphorus contained in runoff from disturbed areas due to phosphate mining activities in the Peace River Watershed. The experiment is located in Bartow, Florida at 27° 48' 45.76"N and 81° 47' 41.81"W. Each experimental site had a set of four source areas and filter strips, for a total of 8 paired source area-vfs plots. Source areas were maintained by cleaning periodically the soil without disturbing the topography. The filter strips were frequently mowed in order to have optimal conditions for sediment trapping and water infiltration.

In order to study different conditions of slope, VFS length, hydraulic conductivity and Source Areas-VFS ratios (2.5:1 and 1.25:1). One experimental site was installed on a flat terrain located close to the Peace River, and the other one was located on a small hill. They are referenced as “River” (or A) and “Hill” (or B) sites in this document (see Figure 4-1). The distance between both plots is approximately 0.85 miles. The dimensions and instrumentation of the experimental plots are shown in Figure 4-2. Each plot, either source area or filter strip, is separated by plastic plates inserted vertically to avoid lateral runoff losses or interference between plots.

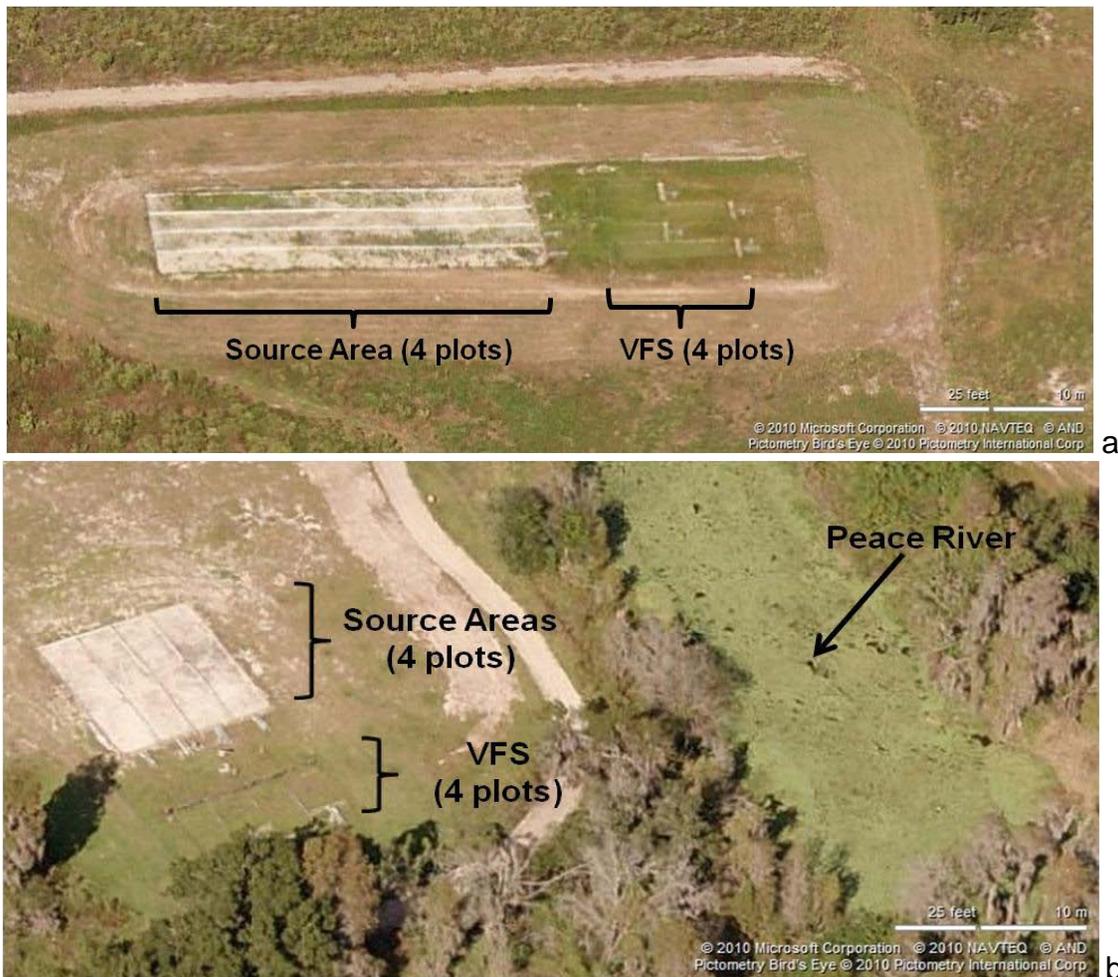
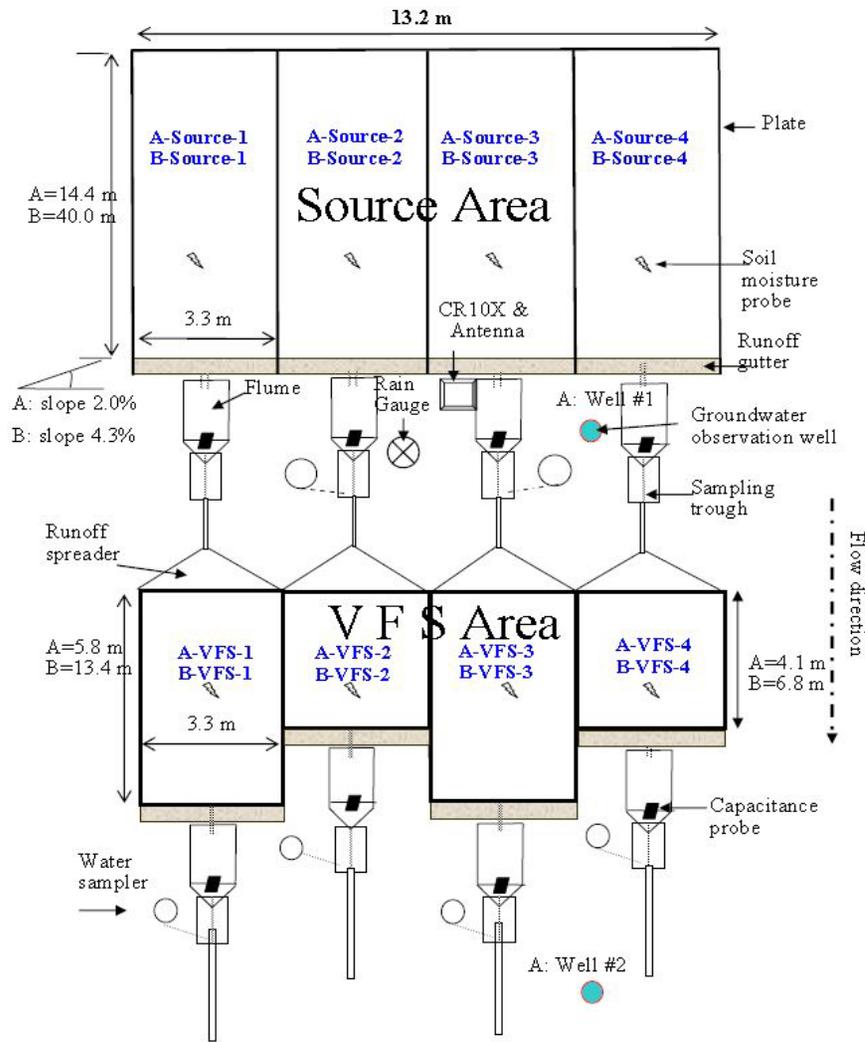
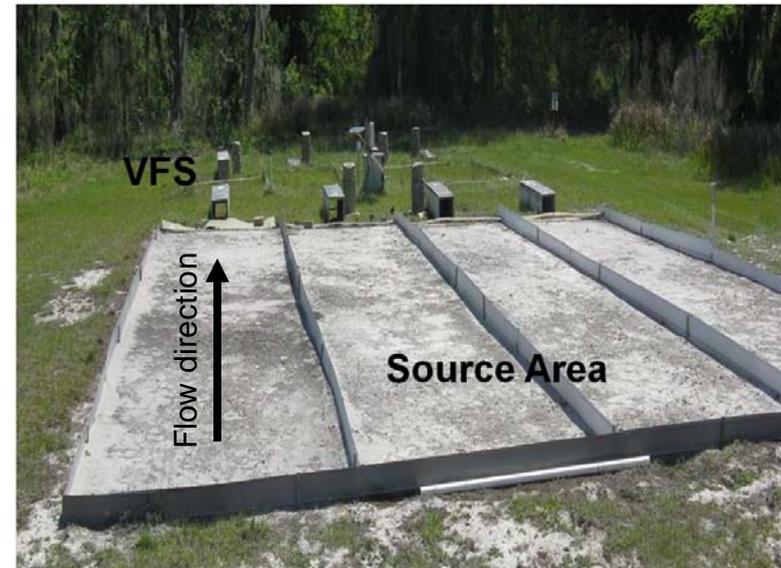


Figure 4-1. Aerial views of the experimental sites located in Bartow, Florida. Figure a corresponds to the “Hill” experimental site, Figure b shows the “River” experimental site. Source: Microsoft ® Bing maps (as accessed on June, 2010).



a



b

Figure 4-2. Schematic dimensions and instrumentation of the experimental sites (Figure a), where letter “A” refers to the “River” site and “B” to the “Hill” site. Figure b shows a picture of the “River” site plot. Source: Kuo (2007).

When an excess rainfall event occurs, runoff is produced from the source areas into the VFS. Runoff is collected in both, at the end of source areas and VFS and directed to six-inch (15.24 cm) HS flumes, where flow rate is automatically measured using capacitance probes (ECH2O, model EC-20, Decagon Devices, WA) inserted vertically into the throat of each flume. At this point water samples are taken using the ISCO 6712 automatic water sampler (ISCO, Inc.) which collects up to 500 ml of sample based on changes in accumulated runoff volume. Another capacitance probe was used to measure soil moisture in periods of 30 minutes. To measure rainfall intensity, a rain gauge (Texas Electronics, Inc TR-525M tipping bucket rain gauge) was installed in both experimental sites. The rainfall data was recorded every minute. All the reading from probes were sent to the CR-10X data logger through a relay multiplexer (AM416, Campbell Scientific, UT). There was a data logger for each site.

Additional details on the procedure and instrumentation of data collection and analysis of water flow, sediment and phosphorous concentrations can be found in Kuo (2007), Kuo and Muñoz-Carpena (2009) and Kuo et al. (2009).

4.3 Experimental Results

Experimental results for years 2005 to 2006 can be found in Kuo (2007). Tables B-1 to B-6 in the Appendix B summarizes the data collected in 2007 and 2008 for rain, runoff, i_{30} , Total Load of Sediments, Total Phosphorus (TP) and Dissolved Phosphorus (DP) for both field sites River (A) and Hill (B) following the same structure as presented by Kuo (2007).

Rainfall excess is in generally produced at the experimental sites when reasonably large rainfall events occurs with intensities above $i_{30} = 10-14$ mm/h for Sites B and A respectively. Data of precipitation was well recorded in the River Site, except during

August 2007 and half of September 2007 because malfunctioning of the CR10 data logger, which was substituted for a new one.

A large number of rainfall events were recorded at the Site A in 2007 (thirty-three in total), unfortunately only 19 of them gave an $i_{30} > 14$ mm/hr to obtain runoff (55%). Five events out of nineteen occurred during the maintenance period and five more during the months of August and September, when the data logger failed (Table B-1). No significant rainfall event was recorded for January, November and December 2007. During the period January – April in 2008, we recorded five events with an $i_{30} > 14$ mm/hr. Three of them with an $14 < i_{30} < 16$ mm/hr produced enough runoff, but the water samplers did not work properly and no water sample was collected for chemical analysis. Two more events ($i_{30} > 25$ mm/hr) collected enough water sample in the 500ml water bottles for P and sediment chemical analysis.

Due to the physical conditions of the Hill site (greater slope, area mainly) more maintenance work was needed because the flumes were frequently clogged with sediment. On the other hand, it was observed that grass grew faster in site A compared to site B. Due to the frequent maintenance of site B, rainfall was missed. In order to estimate the i_{30} it was necessary the adoption of rainfall data from sources other than the local rain gauge. When this particular situation happened, data was provided by the Bureau of Mining Reclamation at Bartow. One thing that is important to point out is the fact that the reports provided by the Bureau estimated the rainfall in inches, with a minimum of 0.01 inch (0.254 mm) every 5 minutes. This data (0.254 mm) is greater than the minimum value that the rain gauge at the site can record (0.1 mm).

The rainfall intensity (i_{30}) at Site B was evaluated based on both: field data when available and from the reports of the Mine Reclamation Bureau. For this site, we estimated that a total of 54 events may be happened in 2007; however 38 of them reported and $i_{30} < 10$ mm/hr, which represents 68% of the total. In summary, from the 54 possible rainfall events, just 16 produced enough rainfall excess. Since many of these events occurred during the maintenance period of the site, only six events had all the conditions needed for water sample collection. From these 6 events, the automated water sample system worked and sample water for chemical analysis for five events, missing only one. For year 2008, up to 17 rainfall events occurred in this site, but only 4 were and an $i_{30} > 10$ mm/hr. in fact, the equipment collected enough water samples in two different events: February 23 and April 06.

Tables B-5 and B-6 in the Appendix B summarize the results for the water samples collected in sites A and B. Data is presented as load of sediments (Sed), total phosphorus (TP) and dissolved phosphorus (DP) in grams. Source areas 1 and 4 (See Figure 3-2a) are always reported with zeros because there are no water samples located on those plots. Six automatic water samplers are installed in each field site, distributed as seen on Figure 3-2.

Table B-7 shows a summary of balances of water, sediments, TP and DP during the period of analysis January 2007 – April 2008. Values of variables related to rain (rainfall duration, total rainfall and i_{30}) may be underestimated because they are obtained from different sources (site and those provided by the Bureau) and which can alter the water balances for a storm by storm basis analysis. Despite those considerations, Table

B-7 shows that more water and pollutants (sediments, total phosphorus and dissolved phosphorus) are obtained in the site B (Hill).

A rainfall event occurring on July 07th, 2006 on the River Site A, plot 2, was selected to simulate the transport of dissolved phosphorus from phosphate mining areas in vegetative filter strips (Kuo, 2007). Data from the experimental river site A is preferred over those of site B (Hill) for testing purposes because the sediment load coming from the source area is lower. Since Kuo (2007; Kuo et al., 2009) reported that phosphorus can be released to runoff from soil (or sediments) based on apatite dissolution, then the presence of sediments could increase the sources of phosphorus in runoff which would add complexity to the system.

4.4 Model Inputs and Sensitivity Analysis

4.4.1 Hydrological and Water Quality Data

Experimental results reported by Kuo (2007) will be used to calibrate the hydrology part of VFSSMOD-W before running the flexible water quality module for the simulation of dissolved phosphorus in runoff from soil based on the rainfall event of July 07th, 2006 on the River Site A, plot 2, named A070706R2. The set of hydrological parameters used in VFSSMOD-W is listed in Table A-10. Values of initial water content (θ_i), filter width (FWIDTH), filter length (VL) and Manning coefficient in the VFS (RNA) were estimated using the inverse calibration module of VFSSMOD-W.

Hydrographs for A070706R2 event are shown in Figure 4-3. An output measured hydrograph (solid dots) as reported by Kuo (2007) is compared to a simulated outflow hydrograph (bold solid line) from VFSSMOD-W. The simulated outflow hydrograph reproduces the shape of the input hydrograph but loses the first section of the observed outflow hydrograph, which starts around 900 seconds and also missed the tail. The Nash-

Sutcliffe coefficient was 0.71 and the simulated outflow was able to capture the two peaks of this rainfall event.

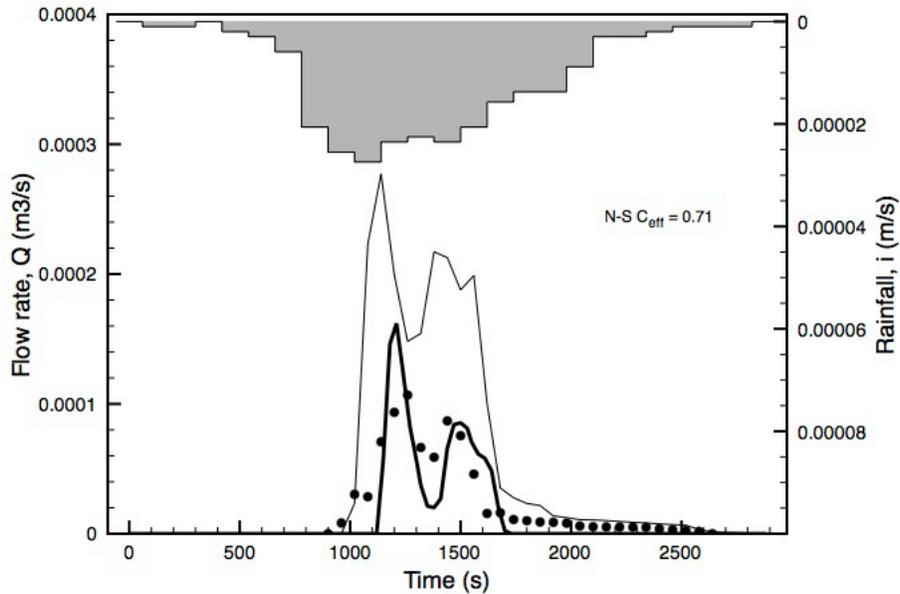


Figure 4-3. Observed and predicted output and input hydrograph for event A070706R2.

Concentration of dissolved phosphorus is reported by Kuo and Muñoz-Carpena (2009) as pollutographs (load of pollutants with time) at the entrance and exit of the VFS. Kuo (2007) reported up to 66% removal of dissolved phosphorus mass due to the used of VFS for the experimental sites A and B. In 2009, Kuo et al. (2009) presented a simplified model where the inflow and outflow dissolved phosphorus concentration can be considered approximately equal. These two findings, reduction of 66% and similar concentration in inflow and outflow, are used as reference when calculating the mass balances of DP in runoff.

Based on the incoming hydrograph and pollutograph reported by Kuo (2007), an estimated input concentration of 0.38 mg/l of dissolved phosphorus is calculated. Figure 4-5 shows the experimental and simulated values of concentration of dissolved phosphorus at the exit of the VFS.

4.4.2 Chemical Conceptual Model

Kuo et al. (2009) investigated the factors that control the release of phosphorus to runoff in phosphate mining areas. They found that soils contain high concentrations of apatite as a source of phosphorus in mining areas, and that the phosphorus is released from apatite by the effect of dissolution. Dissolution is controlled by various factors such as the specific surface area of a particle SSA_{CFA} , the pH in surface runoff, the dissolution rate constant k_a , and the bulk density ρ_b and porosity η of the soil. The dissolution rate of apatite from soil K_{CFA} , in $\text{mg L}^{-1} \text{s}^{-1}$, is given by:

$$K_{CFA} = 31K_a[H^+]^n SSA_{CFA} \frac{\rho_b}{\eta} \quad (4-1)$$

The SSA of the apatite (CFA) per gram soil (m^2g^{-1}) can be calculated as follows:

$$SSA_{CFA} = \sum_{i=1}^n \left(\frac{\text{Particle Size}(i) * P \text{ concentration}(i)}{0.158} \right) * \overline{SSA_{CFA(i)}} \quad (4-2)$$

where *Particle Size (i)* represents the fraction of particles in a particular size range (*i*), *P concentration (i)* is the phosphorus concentration within a given particle size range (*i*) in mg/kg ; $\overline{SSA_{CFA(i)}}$ is the specific surface area for a given particle size range (*i*) in m^2/g ; the P fraction per unit weight of apatite is 0.158 from the formula

$\text{Ca}_{9.62}\text{Na}_{0.273}\text{Mg}_{0.106}(\text{PO}_4)_{4.976}(\text{CO}_3)_{1.024}\text{F}_{2.41}$, which corresponds to Carbonate Fluor Apatite or CFA. Values of SSA_{CFA} for the experimental site were in the ranges 0.00868 – 0.1119 $\text{m}^2 \text{g}^{-1}$ for the River Site A, and 0.01256 – 0.01446 for the Hill Site B $\text{m}^2 \text{g}^{-1}$ (Kuo, 2007; Kuo et al., 2009).

Kuo (2007) reported that dissolution of apatite can only occur when the concentration of dissolved phosphorus in runoff is lower than the equilibrium phosphorus concentration (EPC_0), which was determined to be at 15 mg/l . He also reported that

when runoff phosphorus concentration is higher than EPC_0 , phosphorus is absorbed to soil or sediments. Experimental data reports by Kuo (2007) for years 2006 and 2007, and the extended period 2008-2009, did not show concentrations of dissolved phosphorus greater than 1 mg/l for experimental River Site A, or 5 mg/l for Hill Site B.

In order to account for the factors involved in the transport and reaction of apatite in VFS, a conceptual model needs to be designed. Figure 4-4 shows the elements to include for understanding the transport of phosphates in VFS, where C_w and C_{pw} represents the concentration of phosphorus in surface runoff and porewater respectively, i represents the infiltration rate, and K_{CFA} is the rate of phosphorus dissolved from apatite. The variables q , C and v correspond to the flow, concentration of phosphorus and flow velocity at different positions in the filter strip.

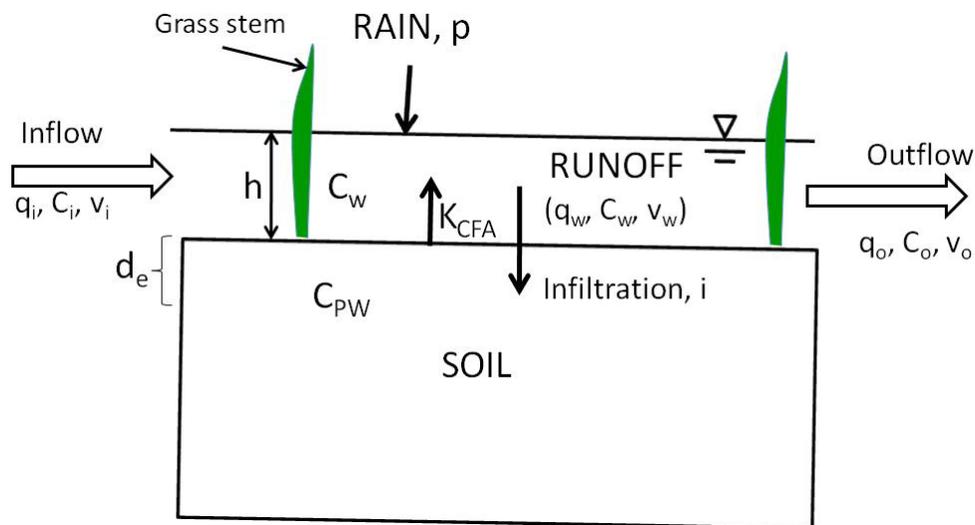


Figure 4-4. Conceptual model for the simulation of soluble phosphorus in VFS for phosphate mining areas.

VFSMOD-W accounts for the effect of pollutant runoff dilution by rain through its transport component as described in previous chapters. The release of apatite from soil and the loss can be represented by the following equation based on Figure 4-4.

$$\frac{dC_w}{dt} = K_{CFA} \quad (4-3)$$

When pH is used to approximate $[H^+]$, equation 4-3 is transformed to

$$\frac{dC_w}{dt} = 31K_a(10^{-pH})^n SSA_{CFA} \frac{\rho_b}{\eta} \quad (4-4)$$

There is no need of a system for coupled of ODE to describe the dynamics of phosphate in runoff since the concentration of dissolved phosphorus in runoff is always lower than the EPC_0 (no absorption of DP to soil) and that the return of dissolved phosphorus contained in porewater soil to runoff is a process not considered or experimentally reported to occur. Table A-11 contains the parameters used for simulating the A070706R2 event.

4.5 Model Testing

The transport of dissolved phosphorus in VFS will be simulated based on two scenarios:

1. Transport of phosphorus considering the effect of dilution from rain but without dissolution from apatite.
2. Same as 1, but including the effect of apatite dissolution from soil.

Based on a simplified model of the transport of dissolved phosphorus in VFS, Kuo and Muñoz-Carpena (2009) found that the concentration of dissolved phosphorus can be considered equal in the inflow and outflow and that for this experimental site, up to 66% of DP removal is expected (Kuo, 2007). Moreover, they (Kuo and Muñoz-Carpena, 2009) conclude that the field scale experimental results in outflow cannot be explained by only considering the transport of phosphorus in runoff, the effect of dilution by rain, and the infiltration. At the end, one of the most important conclusion of their work was

that the outflow concentration of dissolved phosphorus can be explained when the phosphorus coming from apatite dissolution is incorporated in the analysis.

Simulated results for both scenarios are compared to experimental results for concentration and loads (Figure 4-5 and 4-6). A basic sensitivity analysis is performed in order to investigate how each effect of each factor of Equation 4-1 affects the dissolution rate of apatite in runoff K_{CFA} .

For simulating the first scenario, the values for the longitudinal dispersivity and the diffusion coefficient for phosphorus in water were 0.1 m and $8.4 \times 10^{-10} \text{m}^2/\text{s}$ (Kadlec and Wallace, 2008) respectively.

In order to perform the simulation using the flexible water quality module of VFSSMOD-W, two input files need to be included: The A070706R2.iwq (Table A-12) and the Bartow.XML input files (see Appendix A). The structure of these input files follow the format presented in the section “Water Quality Input File Structure for VFSSMOD”, in Appendix A. The values of the parameters used in Equation (4-4) are found in Table A-11 in Appendix A.

4.5.1 Effect of Apatite Dissolution in Runoff

Simulation results for scenarios 1 and 2 confirm the findings of Kuo and Muñoz-Carpena (2009): The sole transport and dilution of dissolved phosphorus in runoff cannot reproduce the outflow concentration, but the incorporation of the phosphorus coming from soil via apatite dissolution allows a removal of 63% the dissolved phosphorus coming in runoff (see Table 4-1), as reported by Kuo (2007).

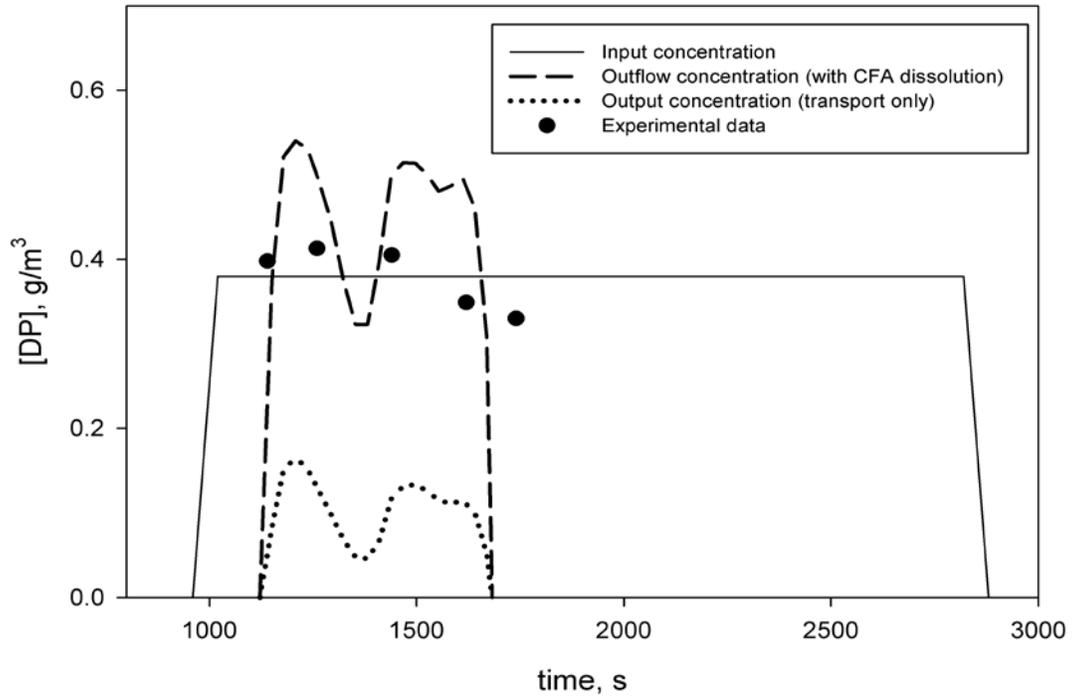


Figure 4-5. Simulated results for the transport of dissolved phosphorus concentration considering the effect of apatite dissolution.

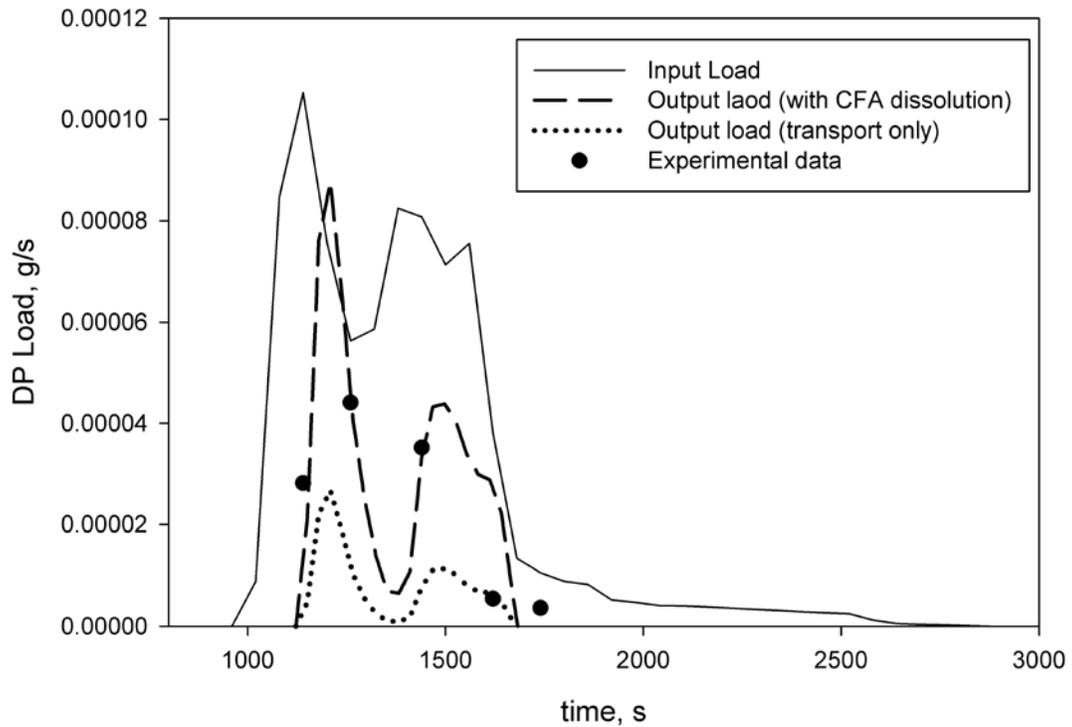


Figure 4-6. Simulated results for the transport of dissolved phosphorus load considering the effect of apatite dissolution.

The only adjustment made in Equation (4-1) with respect to the original values reported by Kuo (2007) was the reaction order n , from -0.67 to -0.823. The rest of the parameters remained unchanged. In the next section, a basic sensitivity analysis is performed to identify the most critical parameters for the dissolution of CFA from soil to runoff.

Table 4-1. Water Balance and phosphorus balances for event 070706R2.

	Experimental data	Simulated data	Mass balance error (%)
INFLOWS			
Runoff volume*, m ³	0.1297	0.1297	-
DP mass, g	0.0504	0.0504	-
OUTFLOWS			
Runoff volume*, m ³	0.376	0.476	21
DP mass including dissolution of CFA, g	0.01840	0.01831	0.5
DP mass (transport only), g	0.01840	0.0046	75
DP removal Efficiency			
Transport only	63%	75%	+12%
Considering CFA dissolution	63%	63%	-

4.5.2 Sensitivity Analysis of Phosphorus Release From Apatite

A sensitivity analysis of the different parameters involved in the estimation of K_{CFA} is presented here. This analysis has the purpose of identifying those parameters that affect the amount of phosphorus released from apatite to runoff based on equation 3-1. Values reported in Table A-11 are varied by -50, -25, +25 and 50 percent. Due to the wide range of variation between the parameters K_a , SSA_{CFA} , ρ_b and η with respect to n and pH, results are shown in two Figures (4-7 and 4-8)

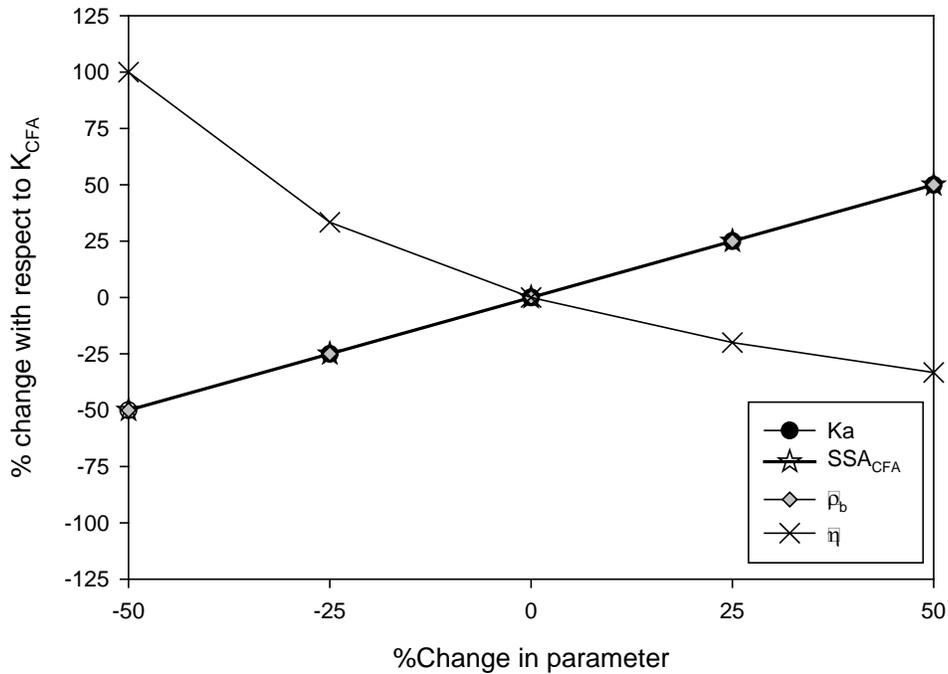


Figure 4-7. Percentile change of K_{CFA} due to variations of K_a , SSA_{CFA} , ρ_b and η .

Variation in parameters K_a , SSA_{CFA} , ρ_b and η affect K_{CFA} in the same proportion, from -50 to +50%. This is because the linearity of these parameters in Equation 4-1. On the other hand, η inversely affects the value of K_{CFA} compared to K_a , SSA_{CFA} , ρ_b and η . Again, from Equation 4-1 we can observe that η is the only parameter that divides this equation.

The major variations of K_{CFA} occurred for a change of +25% and +50% in the parameters n and pH . An exponential trend is observed in Figure 4-8 which is concordant with equation 4-1 because n and pH are included as power functions. When pH is increased for the sensitivity analysis (Figure 4-8), those values resulting from increasing pH in +25% and +50% are beyond the range of validity ($pH > 7$) for the rate constant K_a (Kuo, 2007). However, the purpose of this section was to show how sensitive K_{CFA} is with respect to the change of its parameters.

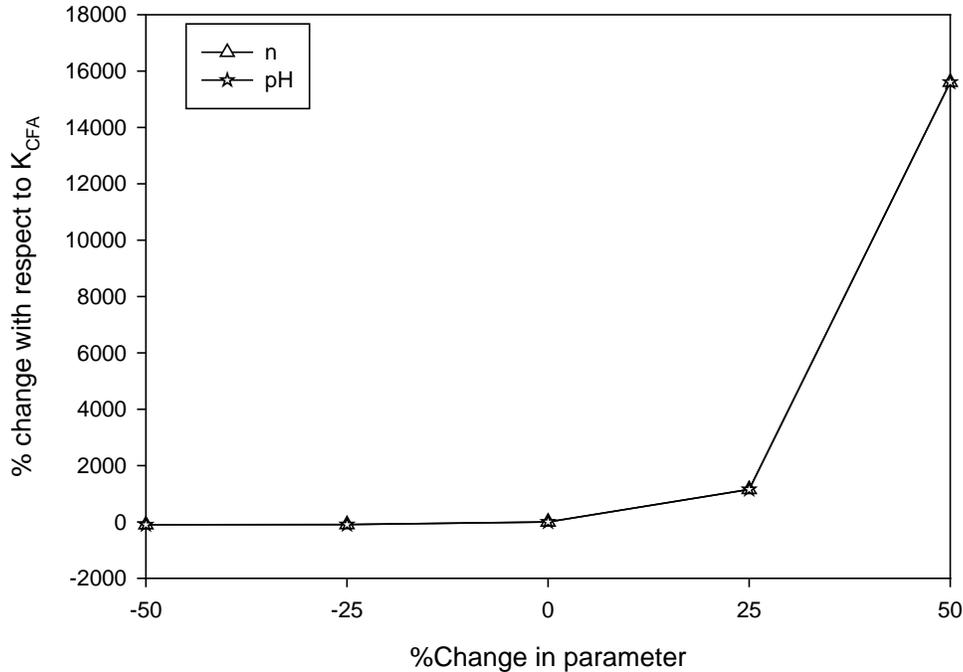


Figure 4-8. Percentile change of K_{CFA} due to variations of n and pH .

4.6 Discussion of Results

The selection of the rainfall event A070706R2 was appropriate in order to simplify the conceptual model to be used for the simulation of dissolved phosphorus in runoff coming from phosphate mining areas when VFS are used. By choosing this event, the influence of phosphorus dissolution from apatite contained in sediments was lowered, and the analysis was focused only on the effect of dissolution of apatite from soil within the vegetative filter strip.

Results showed that experimental bromide load and concentration cannot be explained by the solely transport of dissolved phosphorus through the VFS (See Figure 4-5 and 4-6). The infiltration and dilution from rain are the two major factors affecting the concentration in this scenario.

When dissolution of CFA is taken in consideration, the model can approximated the reported values con DP concentration, except for one point (Figure 4-5) and can

predict the total mass of dissolved phosphorus at the end of the VFS (Figure 4-6 and Table 4-1) as reported by Kuo (2007) based on the loads of dissolved phosphorus. From Figure 4-6 we can observe that the missed concentration point by the simulation corresponds to the tail, and that this has very little effect in terms of DP load.

By making a mass balance between the amounts of DP that exits the VFS with and without the apatite dissolution (Table 4-1), we can say that for this case the VFS could remove up to 75% of the incoming runoff DP, but the effect of apatite dissolution adds DP to runoff so the final efficiency is 63%. Dissolution of apatite helps to explain the little change in runoff water between the inflow and outflow during the simulation at some points (Figure 4-5)., however, is likely that lower concentrations were not observed due to the inability of the equipment to collect water samples under flow conditions.

Without considering the dissolution of CFA, is not possible to explain the DP removal efficiencies reported by Kuo (2007). Additionally, the concentration of dissolved phosphorus decreases due to the effect to dilution by rain to an average concentration lower than 0.15 mg/l (Figure 4-8).

Water also impacted in the outflow load for mass balances. In Figure 4-3 we observed that the simulated hydrograph over-estimated the first pick, but misses the tail. This overestimation allows balancing the mass phosphorus in the outflow, without considering the long tail. The overestimation of the first runoff pick compensates the lack of a tail in the simulated data.

One of the most influential factors that contributed to adjust the averaged output concentration and DP outflow load was the reaction order, n , in equation 4-1, as seen

during the sensitivity analysis performed in section 4.5.2. This analysis helped in understanding the reason why a slight change in parameter n greatly affects the outflow runoff concentration of dissolved phosphorus. Since n and pH are used as the powered part of equation 4-1, a slight increment in these parameters could exponentially modify the amount of phosphorus released from apatite (Figure 4-8). For the rest of the parameters (K_a , SSA_{CFA} , ρ_b and η), the model is also sensitive, but not as sensitive as with n and pH (Figure 4-7).

Finally, it is interesting to point out that the reported experimental concentration of dissolved phosphorus in runoff could be related only to the time where there was enough water in the flume to allow the automatic sample get a water sample. A variation in concentration for low flow might not be observed due to the latter, as predicted using the model (see Figure 4-5). The experience of field work during the extended period (2008-2009) showed that for small rainfall events (I_{30} close to 14 mm/hr) the amount of water samples automatically collected for chemical analysis was minimum and generally sampled at the flow peaks. The fewer samples collected, the less variation in outflow DP concentration can be reported.

4.7 Conclusions

The flexible water quality model of VFSSMOD-W allowed exploring the interactions between the release of phosphorus from apatite dissolution and the loads and concentration of DP in runoff during a rainfall event. The relationship reported by Kuo (2007) for apatite dissolution (Equation 4-1) can help to explain a 66% reduction of DP in this experiment, as reported by Kuo. The sole transport and rainfall dilution of DP was not enough to explain outflow DP loads and concentrations.

The incorporation of Equation 4-1, which is not a linear equation but an exponential one, in the analysis of how the dissolved phosphorus is transported in runoff was a good opportunity to test the flexible transport and reactive module of VFSSMOD for other conditions different to those linear and Monod kinetics used during the analytical testing of the module.

Parameters have to be wisely selected to represent the dissolution of apatite in runoff because Equation 4-1 is highly sensitive to parameters variation, especially for increases on n and pH . The pH is another factor to consider since the validity of parameter k_a depends on the value of pH (Kuo, 2007).

The model not only can handle different formulas to describe the dynamics of pollutants in runoff in VFS, but the more important and exciting part is the fact that those formulas can finally be related to physically based phenomena developed for each particular pollutant. The potential of this tool can help to explore new theories for removing pollutants in VFS, or simply test the existing theories to help the researchers and decision making personnel evaluate the efficiency of VFS.

CHAPTER 5 CONCLUSIONS

5.1 General Conclusions

A novel flexible numerical model to simulate the transport of runoff pollutants through vegetative filter strips was successfully tested with different analytical solutions and coupled to the program VFSSMOD-W to simulate the transport of runoff pollutants under dynamic flow conditions. In this flexible approach, the user is able to define the processes and relationships involved in the transport of pollutants in surface runoff by the use of a conceptual model.

Analytical testing included the evaluation of several numerical techniques to determine the best method for coupling with VFSSMOD-W as a flexible water quality module. The alternating TRT split operator method was selected to be coupled to VFSSMOD-W because it produced the lowest error (L^2 error norm) for the different scenarios tested during the evaluation process.

The new flexible module of VFSSMOD-W was used to analyze the transport of bromide in runoff over a sand bed under controlled laboratory conditions. Three different user-defined conceptual models were evaluated in order to predict the outflow concentration of bromide. The two conceptual models that better approximated the experimental results were based on an empirical uptake/release approach and a physically based approach based on the exchange layer theory (Gao et al., 2004). Despite the fact that these two approaches had high values Nash-Sutcliffe coefficient (>0.94), the mechanistic approach can be applied to other set of experimental data while the parameters of the empirical approach is limited to those conditions of the experiment.

The flexible multi reactive transport component of VFMOD-W was also tested with data from a field scale experiment where runoff phosphorus is produced from phosphate mining tailing areas and is removed by using VFS (Kuo, 2007; Kuo et al., 2009). Kuo (2007) reported a 66% removal efficiency for dissolved phosphorus in his experiment. A conceptual model that considers the dissolution of apatite (Kuo et al., 2009) was developed and tested with the experimental data to explore the processes involved in the transport of dissolved phosphorus in surface runoff. Again, the use of a user-defined conceptual model parameterized with physically based processes allowed us to explore and explain the processes involved in the removal of dissolved phosphorus in runoff.

The flexible water quality module of VFMOD-W opens a new window of possibilities to study the transport and reaction of pollutants under dynamic conditions in surface runoff. The program is open to the incorporation of future theories for a wide variety of pollutants (i.e. chemical, biological, nanoparticles) and field conditions, but the user must develop the conceptual model that is driving the dynamics of pollutant within the filter strip. The implementation of a mechanistic approach for estimating the removal of runoff pollutants through vegetative filter strips could also help researchers, consultants, agencies and other people to find the optimal characteristics of the VFS (i.e. length) without the use of the limited empirical approach, which is constrained to the field conditions for which the empirical equations were developed.

5.2 Limitations

The current version of the flexible module is limited to one mobile component (i.e. solute) that can be interacting with various stable components (i.e. vegetation, sediments, soil, porewater, etc), which limits the level of complexity that can be handled.

The building of the conceptual model for each species of pollutant to evaluate is the most challenging part of the flexible approach, and requires a knowledgeable user in the processes that drive the pollutant transport. The implementation of the XML input file can be challenging for first time users. The XML file contains the equations produced with the help of the conceptual model using the nomenclature for XML documents.

5.3 Future Research

Short-term future research topics can be summarized in the next list.

- Testing pollutant interactions between sediments and runoff based on the experimental set of data collected for the field scale experimental site in Bartow, Florida.
- Increase the number of mobile components to simulate multiple-species transport in runoff through VFS.
- Model testing with more complex pollutants (i.e. nanoparticles, pathogens).
- Collaborate with other researchers to explore new theories, such as the theories evaluated in this work: the exchange layer theory (Gao et al., 2004) or the dissolution of apatite (Kuo, 2007; Kuo et al., 2009).
- Perform a global sensitivity and uncertainty analysis of the conceptual models.

APPENDIX A. INPUT FILES FOR ANALYTICAL AND EXPERIMENTAL TESTING

This appendix contains the following information:

- Twelve tables referenced in chapters 1, 2 and 3 for the structure of the input files needed to run the stand alone transport component the coupled program TRT-VFSMOD for simulating the transport of bromide and phosphorus in runoff through VFS. Information about the parameters used for the simulation with VFSMOD is also available here.
- Full detailed analytical solutions (van Genuchten, 1982) for scenarios I-III used in chapter 1 for conservative a reactive solute.
- Full description of the water quality input file used in VFSMOD for using empirical simulation of pesticides (Sabbagh et al., 2009), transport of a conservative solute and the use of the flexible multi-reactive module based on RSE.
- Input files used in VFSMOD-W to simulated the transport of bromide used in chapter 2 and the transport of phosphorus from chapter 3.
- XML input files used to test the flexible component in the RSE, TRT modules
- XML input files used to simulate the transport of bromide used in chapter 2 and the transport of phosphorus from chapter 3. This input files are recalled from the VFSMOD-W projects

Tables A-1 to A-12

Table A-1. Parameters for femadr.in input file

Parameter	Description
L	Total length of the domain in the X direction (parallel to flow), [Length].
DX	Spatial discretized length in the X direction, [Length].
VX	Flow velocity in X direction, [Length/Time].
DISL	Longitudinal dispersivity, [Length].
DISM	Molecular diffusion coefficient, [Length ² /Time].
THETAW	Time weighting method for the temporal derivative (0.5 for Crank-Nicholson), [Dimensionless]
K ₁	First order decay reaction coefficient, [1/Time].
DT	Time step, [Time].
NDT	Number of time steps for the simulation
NL	Order of the integration rule over each element
NPOL	Number of nodal points over each element

Table A-2. XML input file equation structure for describing a simple uptake/release model. Adapted from James (2008b)

```

<equations>
  <equation>
    <lhs>water_column_p</lhs>
    <rhs>-k_u*water_column_p + k_r*settled_p/depth</rhs>
  </equation>
  <equation>
    <lhs>settled_p</lhs>
    <rhs>depth*k_u*water_column_p - k_r*settled_p</rhs>
  </equation>
</equations>

```

Note: k_u is k_{st} and k_r is k_{rs} for the system of equations (1-8) and (1-9)

Table A-3. XML input file structure for running RSE

XML tags	Description
Reaction Set	Name of the reaction set to be used during the simulation. The reaction set contains information about stores, variables, parameters and equations.
Coverage	Coverage of the parameters. In TaRSE, parameters can be used by a single cell or for all the 2D mesh. In RSE, only the coverage over the entire domain is available.
Stores	The different stores to be used are defined here.
Components	This tag contains all the variables (mobile or stable) and parameters needed during the simulation, including 22 variables. Values for each variable and parameter have to be declared, but they won't be read from here as input data for RSE. A text file (.iwq) contains the variables to be used along with their corresponding values.
Equations	Equations to be used in the simulation are declared here. See Table A-1 for details.

Table A-4. Example of the *.iwq file structure for running RSE in TR-FEM.

```

2
'wq_input_base.xml' 'component_output_base.xml' 'rs1'
1 water_column_p 100
1 settled_p 0
2 k_u -0.1 k_r -0.05
0
depth 2.2 x_vel_ol 0 time_step 3600 area 0

```

Table A-5. Description of the *.iwq input file used to test the TR-RSE and TRT split operator programs.

```

2
'wq_input_base.xml' 'component_output_base.xml' 'rs1'
1 water_column_p 100
0 settled_p 0
1 k1 -0.1
0
depth 2.2 x_vel_ol 0 time_step 3600 area 0

```

Table A-6. Description of the *.iwq file when the fully coupled finite element method is used to simulate the transport and reaction of a pollutant in surface runoff.

```

2
25 0.5 .01 0.0

```

Table A-7. Description of the *.iwq file when the TRT_RSE module is used to simulate the transport and reaction of a pollutant in surface runoff.

```

3
'sample.xml' 'sample_index_out.xml' 'rs1'
1 water_column_p 100 0.1 2.08E-9 0
1 porewater_p 0
2 k_st 0.1 k_rs 0.016
0

```

Table A-8. Description of the water quality input file sampleBr.iwq

```

3
'YuGao.xml' 'component_output_YuGao.xml' 'rs1'
1 water_column_p 103 0.03 2.08E-9 0
1 porewater_p 0
5 er .3E-6 h 0.000257 inf 0.000011681 de 0.3 alpha 0.9
0

```

Table A-9. Hydrological input factors used by VFMSOD-W to simulate the mass water balance of outflow runoff and infiltrated water.

Hydrological input (units)	Value	Description
FWIDTH (m)	0.402	Effective flow width of the strip
VL (m)	1.52	Length in the direction of the flow
RNA*(sm ^{-1/3})	0.0101676	Filter Manning's roughness n for each segment
SOA* (m/m)	0.0204230	Filter slope for each segment
VKS* (ms ⁻¹)	1.18646X10 ⁻⁵	Soil vertical saturated hydraulic conductivity in the VFS
SAV* (m)	0.116654	Green-Ampt's average suction at wetting front
OS (m ³ m ⁻³)	0.453	Saturated soil water content, θ_s
SHCK (-)	0	Relative distance from the upper filter edge where check for ponding conditions is made (i.e., 1 = end, 0.5 = midpoint, 0 = beginning)

* Optimized values.

Table A-10. Hydrological parameters used in VFDSMOD-W for A070706R2 event.

Parameter (units)	Value	Description
FWIDTH (m)	1.5	Effective flow width of the strip
VL (m)	4.39	Length in the direction of the flow
RNA(sm ^{-1/3})	0.048	Filter Manning's roughness n for each segment
SOA (m/m)	0.018	Filter slope for each segment
VKS* (ms ⁻¹)	0.00004074	Soil vertical saturated hydraulic conductivity in the VFS
SAV (m)	0.1	Green-Ampt's average suction at wetting front
OS (m ³ m ⁻³)	0.45	Saturated soil water content, θ_s
OI (m ³ m ⁻³)	0.4164	Initial soil water content
SM (m)	0	Maximum surface storage
SHCK (-)	0	Relative distance from the upper filter edge where check for ponding conditions is made (i.e., 1 = end, 0.5 = midpoint, 0 = beginning)

Table A-11. Apatite dissolution parameters used in VFDSMOD-W for A070706R2 event.

Parameter (units)	Value	Description
Ka (moles m ⁻² s ⁻¹)	6.91X10-8	Dissolution rate constant
n (dimensionless)	-0.823	Reaction Order
SSA _{CFA} (m ² g ⁻¹)	0.1066	Specific surface area of CFA
pH (dimensionless)	6.1	Potential of Hydrogen
ρ_b (g cm ⁻³)	1.38	Soil bulk density
η (cm ³ cm ⁻³)	0.47	Porosity

Table A-12. Description of the water quality input file Bartow070706R2.iwq

3
 'Bartow.xml' 'component_output_Bartow.xml' 'rs1'
 1 water_column_p 0.38 0.045 8.4E-10
 0 porewater_p 0
 6 Ka 6.91E-8 n -0.823 SSA 0.01066 pH 6.1 db 1.38 POR 0.47
 0

Analytical Solutions

Input Pollutant Concentration as a Pulse and Continuous Without Reactive Term.

Governing equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x}$$

Initial and boundary conditions

$$C(x,0) = C_i = 0$$

$$C(0,t) = \begin{cases} C_o & 0 < t < t_o \\ 0 & t > t_o \end{cases}$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

Analytical solution:

For $0 < t < t_o$

$$C(x, t) = C_i + (C_o - C_i) A(x, t)$$

For $t > t_o$

$$C(x, t) = C_i + (C_o - C_i) A(x, t) - C_o A(x, t - t_o)$$

where

$$A(x, t) = \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt}{2(Dt)^{1/2}} \right] - \frac{1}{2} \exp \left(\frac{vx}{D} \right) \operatorname{erfc} \left[\frac{x + vt}{2(Dt)^{1/2}} \right]$$

NOTE: For continuous input of pollutant, make t_o equal to time of simulation.

Input Pollutant as a Function of Time Without Reactive Term.

Governing equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x}$$

Initial and boundary conditions

$$C(x,0)=C_i=0$$

$$C(0,t)=C_a + C_b e^{-\lambda t} \quad \text{with } C_a=80, C_b=30 \text{ and } \lambda=1$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

Analytical solution:

$$C(x, t) = C_i + (C_a - C_i) A(x, t) + C_b B(x, t)$$

where

$$A(x, t) = \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt}{2(Dt)^{1/2}} \right] + \frac{1}{2} \exp \left(\frac{vx}{D} \right) \operatorname{erfc} \left[\frac{x + vt}{2(Dt)^{1/2}} \right]$$

$$B(x, t) = e^{-\lambda t} \left\{ \frac{1}{2} \exp \left[\frac{(v - u)x}{2D} \right] \operatorname{erfc} \left[\frac{x - ut}{2(Dt)^{1/2}} \right] + \frac{1}{2} \exp \left[\frac{(v + u)x}{2D} \right] \operatorname{erfc} \left[\frac{x + ut}{2(Dt)^{1/2}} \right] \right\}$$

And with

$$u = v \left(1 - \frac{4\mu D}{v^2} \right)^{\frac{1}{2}}$$

Input Pollutant Concentration as a Pulse and Continuous with Reactive Term.

Governing equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \mu C + \gamma \quad \text{with } \mu=0.1 \text{ and } \gamma=0$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

Analytical solution:

For $0 < t < t_0$

$$C(x, t) = \frac{\gamma}{\mu} + \left(C_i - \frac{\gamma}{\mu} \right) A(x, t) + \left(C_o - \frac{\gamma}{\mu} \right) B(x, t)$$

For $t > t_0$

$$C(x, t) = \frac{\gamma}{\mu} + \left(C_i - \frac{\gamma}{\mu} \right) A(x, t) + \left(C_o - \frac{\gamma}{\mu} \right) B(x, t) - C_o B(x, t - t_0)$$

where

$$A(x, t) = \exp(-\mu t) \left\{ 1 - \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt}{2(Dt)^{1/2}} \right] - \frac{1}{2} \exp\left(\frac{vx}{D}\right) \operatorname{erfc} \left[\frac{x + vt}{2(Dt)^{1/2}} \right] \right\}$$

$$B(x, t) = \frac{1}{2} \exp\left[\frac{(v - u)x}{2D}\right] \operatorname{erfc} \left[\frac{x - ut}{2(Dt)^{1/2}} \right] + \frac{1}{2} \exp\left[\frac{(v + u)x}{2D}\right] \operatorname{erfc} \left[\frac{x + ut}{2(Dt)^{1/2}} \right]$$

and

$$u = v \left(1 + \frac{4\mu D}{v^2} \right)^{\frac{1}{2}}$$

NOTE: For continuous input of pollutant, make t_0 equal to time of simulation.

Input Pollutant as a Function of Time with Reactive Term.

Governing equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \mu C + \gamma \quad \text{with } \mu=0.1 \text{ and } \gamma=0$$

Initial and boundary conditions

$$C(x,0)=C_i=0$$

$$C(0,t)=C_a + C_b e^{-\lambda t} \quad \text{with } C_a=80, C_b=30 \text{ and } \lambda=1$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

Analytical solution:

$$C(x, t) = \frac{\gamma}{\mu} + \left(C_i - \frac{\gamma}{\mu} \right) A(x, t) + \left(C_a - \frac{\gamma}{\mu} \right) B(x, t) + C_b E(x, t)$$

where

$$A(x, t) = \exp(-\mu t) \left\{ 1 - \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt}{2(Dt)^{1/2}} \right] - \frac{1}{2} \exp\left(\frac{vx}{D}\right) \operatorname{erfc} \left[\frac{x + vt}{2(Dt)^{1/2}} \right] \right\}$$

$$B(x, t) = \frac{1}{2} \exp\left[\frac{(v-u)x}{2D}\right] \operatorname{erfc} \left[\frac{x - ut}{2(Dt)^{1/2}} \right] + \frac{1}{2} \exp\left[\frac{(v+u)x}{2D}\right] \operatorname{erfc} \left[\frac{x + ut}{2(Dt)^{1/2}} \right]$$

$$E(x, t) = e^{-\lambda t} \left\{ \frac{1}{2} \exp\left[\frac{(v-w)x}{2D}\right] \operatorname{erfc} \left[\frac{x - wt}{2(Dt)^{1/2}} \right] + \frac{1}{2} \exp\left[\frac{(v+w)x}{2D}\right] \operatorname{erfc} \left[\frac{x + wt}{2(Dt)^{1/2}} \right] \right\}$$

And with

$$u = v \left(1 + \frac{4\mu D}{v^2} \right)^{\frac{1}{2}}$$

$$w = v \left[1 + \frac{4D}{v^2} (\mu - \lambda) \right]^{\frac{1}{2}}$$

RSE Reactive Module Testing

The RSE testing included the example provided by James (2008b) for a hypothetical simple uptake-release process and, the solution of a system of ODE with an analytical solution.

James (2008b) shows the flexibility of TaRSE with an uptake-release model flowing the example shown in Figure 1-3, but with the next system of equations:

$$\left\{ \begin{array}{l} \frac{dC_p}{dt} = -k_{st} C_p + \frac{k_{rs}}{z_d} S_p \\ \frac{dS_p}{dt} = z_d k_{st} C_p - k_{rs} S_p \end{array} \right. \quad \begin{array}{l} \text{(A-1)} \\ \text{(A-2)} \end{array}$$

where C_p represents the phosphorus in the water column (water_column_p), S_p (settled_p), two reaction coefficients k_{st} and k_{rs} , and z_d is the water depth.

Implementation of the XML input interface is given in Table A-2:

The values used to start the simulation were: C_p : 10 mg/l, S_p : 5mg/m², k_{st} : 0.0001 s⁻¹, k_{rs} :0.000043s⁻¹, depth: 2.2 m and, time step: 3600 s. The total time of the simulation was 36000 s.

Since no analytical solution was found to test this system of equations (eq. A-1 and A-2), the solution was compared with the results obtained using Matlab (ODE4) and a fourth order Runge-Kutta method implemented in a spreadsheet.

A simultaneous system of equations that solves the second order ODE

$$\frac{d^2 y}{dx^2} - y = 0 \quad \text{(A-3)}$$

is used to test RSE. This equation can be solved with the analytical solution $y=\sinh(x)$. The two first order ODE that help us to solve Eq (A-3) are:

$$\frac{dz}{dx} = y \quad (A-4)$$

$$\frac{dy}{dx} = z \quad (A-5)$$

With the initial conditions $y(0)=0$, $z(0)=\left[\frac{dy}{dx}\right]_0 = 0$. The time of the simulation was set to 10 (dimensionless) with $dx=1$.

The Reaction Simulation Engine was first tested as a stand-alone program before being coupled to the transport module of TR-FEM. In the first scenario, a system of two ODE which describe the uptake-release of a pollutant from the water column to the soil is solved using RSE. In a second scenario, RSE solves a simple system of two ODE (which solves a second order ODE). Details of each scenario can be seen previous section. Results of the simulations are shown in Figures A-1 and A-2.

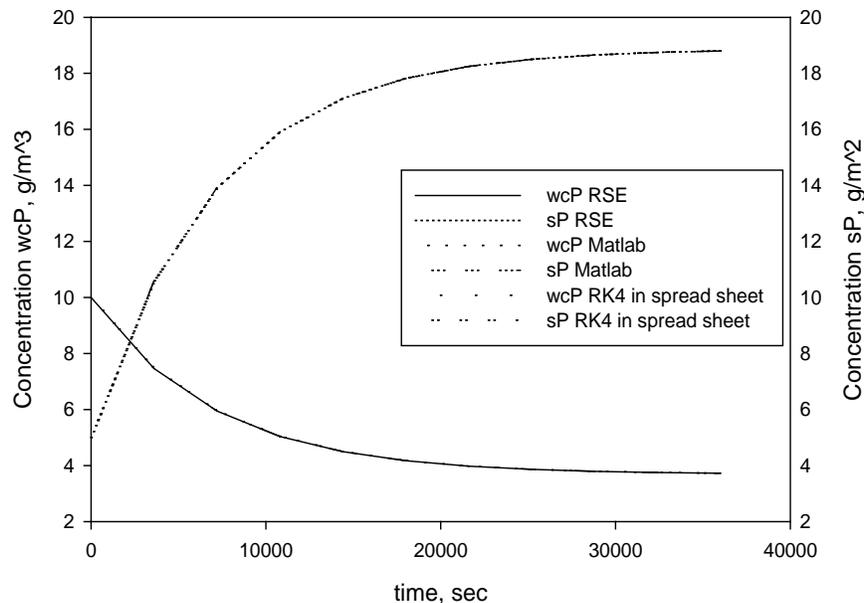


Figure A-1. Comparison of a adsorption-desorption process in a arbitrary node/cell using three different methods: RSE, Matlaboratory (ODE4) and RK4 in MS excel. The maximum difference among them was of the order of $-7.6E-8$ mg/l for wcP and $-1.8E-7$ mg/l for SP. Simulation was run up to $t=36000$ seconds.

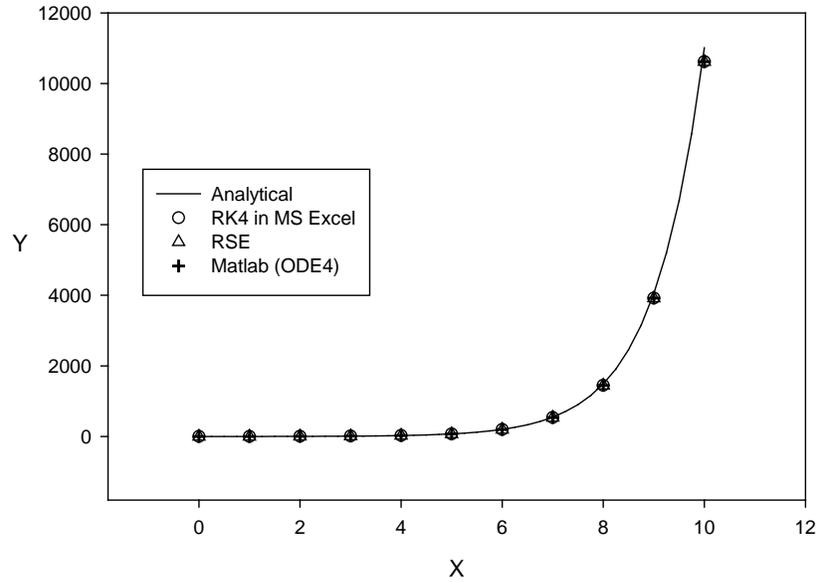


Figure A-2. Comparison of different RK4 methods (MS Excel, RSE, Matlaboratory [ODE4]) to solve the system of ODE equations $dz/dx=y$; $dy/dx=z$ with the initial conditions $y(0)=0$ and $z(0)=1$. The analytical solution $y=\sinh(x)$ comes from solving the partial differential equation $\frac{d^2y}{dx^2}-y=0$ with initial condition $y(0)=0$; $\left[\frac{dy}{dx}\right]_0 = 1 = z(0)$ at $x=0$. The Nash-Sutcliffe efficient coefficient was 0.9984 for the three methods when compared to the analytical solution.

Water Quality Input File Structure for VFSSMOD

The water quality input file (*.iwq) of VFSSMOD has been modified to accept three options: 1) Pesticides based on the empirical equation provided by Sabbagh et al. (2009), which is already included in the current version of the program, 2) The transport of a soluble pollutant with a first order decay kinetics using a the fully coupled finite element method TR-FEM and, 3) The transport and reaction of pollutants using the flexible module TRT. The input file structure for options 2 and 3 is detailed next. Since the first option is already included in VFSSMOD-W and is beyond the scope of this work, it is not depicted. For further information consult the help menu of the program.

Water quality input file structure using the fully coupled finite element method TR-FEM. This option allows the user to estimate the transport and reaction of a pollutant in runoff based on Eq. (2-8). This equation includes the effect of pollutant dilution by rain and is solved using a fully coupled finite element method. The TR-FEM module is nothing else than the transport module of TR-RSE. In this module, the reactivity of the pollutant is limited to a first order decay kinetics ($-k_1C$). Estimation of the pollutant porewater concentration when using this option or other interaction in runoff is not possible. When TR-RSE is used, the decay can be set to coefficient k_1 is set to zero so only the pollutant is though the domain without any reaction.

The *.iwq input file is written in plain text format and contains two lines. In the first line, number 2 indicates that Option 2, fully coupled finite element method, is selected. In the second line the program reads the next four parameters: Soluble pollutant concentration (g/cm^3), longitudinal dispersion coefficient DISL (m), molecular diffusion coefficient DISM (m^2/s) and the first order decay coefficient k_1 (s^{-1}). See Table A-6 for details.

Water quality input file structure using the split operator module TRT. This option allows the user to estimate the transport and reaction of a pollutant in runoff using the flexible module TRT, which has been described in this work. The *.iwq input file contains the next elements:

- In line 1, the number 3 indicates that Option 3, the TRT flexible module is selected,
- Line 2 has three elements: 1) The name of the XML input file where the mobile, stables, parameters, variables and equations are defined, 2) the name of the XML file where the order of the indexes is printed for those parameters defined in the XML input file (currently this file is not needed but produced as a way to corroborate data), and 3) The name of the reaction set of equations to be used by the reactive module of TRT by reading the XML input file.
- The first number of line 3 defines the number of mobile components (i.e. soluble phosphorus) followed by its name, concentration, longitudinal dispersivity, molecular diffusion coefficient and a first order decay coefficient.
- Line four defines the number of stable components (i.e. soluble phosphorus concentration in porewater), followed by its name and initial concentration in the domain.
- Line five defines the parameters and variables used in the reactions set of equations of the XML input file. The first number indicates the number of parameters/variables, followed by pair indicating the name and value.
- The last line is a flag (set to zero) to indicate that the runoff depth, velocity, and time step are taken from VFSSMOD.

Detailed information about the XML input file can be found in James (2008b, c, a).

The key part of the XML input file is the set of equations to be used for the reactive part of the TRT module. The name of the mobile and stable compounds and the variables and parameters used in the equations are defined in the *.iwq file. The program crashes if a variable used in the XML input files has not been defined in the *.iwq file. Table A-7 shows an example of the *.iwq input file with one mobile component, one stable component and two variables.

Some parts of the information in the XML input file may never be used by RSE, but the structure of the file needs to keep all the information in order to ensure compatibility with the way TaRSE reads it. If some information is omitted, a crash is expected to happen. In order to deal with this problem, a second file (*.iwq) is needed when RSE is linked to TR-FEM to input the values of the variables and parameters to be used. Table A-4 shows an example of the input file needed to describe the system of equations shown in Table A-2.

The description of the *.iwq input file is as follows: the first line is a flag for VFSSMOD (Table A-4). The second line has the name of the xml input file (with the structure described in Table A-3), the name of the xml output file generated by RSE to double check the order of the variables and parameters used (this file is not needed to run the program, but is useful for checking internal values of the program during the testing stages), and the name of the reaction set section declared in the xml input file (See Table A-3). In line 3, the first number indicates the number of mobile variables to be used, followed by the name(s) and its value(s). Line 4 is the same as line 3, but for stable components. Line 5 contains the number of parameters to be used, which match with the parameter(s) declared in the reaction(s) (see Table A-2) and the respective value(s). Line 6 is a flag to read the four intrinsic parameters declared in line 7. If the flag is 0, line 7 is not read. If the flag is 1, then it proceeds to read line 7.

Water Quality Project for Bromide Simulation in VFSSMOD

Project File (sampleBrOK0.prj)

```
ikw=inputs\sampleBrOK0.ikw
iso=inputs\sampleBrOK0.iso
igr=inputs\sampleBrOK0.igr
isd=inputs\sampleBrOK0.isd
irn=inputs\sampleBrOK0.irn
iro=inputs\sampleBrOK0.iro
iwq=inputs\sampleBrOK0.iwq
og1=output\sampleBrOK0.og1
og2=output\sampleBrOK0.og2
ohy=output\sampleBrOK0.ohy
osm=output\sampleBrOK0.osm
osp=output\sampleBrOK0.osp
owq=output\sampleBrOK0.owq
```

IKW Input File (sampleBrOK0.ikw)

```
Unit9, g8, u183-91
0.402
1.52 57 .5 .8 350 3 1 1
2
1.2 .0101676 .020423
1.52 .0101676 .020423
1
```

ISO Input File (sampleBrOK0.iso)

```
.0000118646 .116654 .453 .43 0 0
-----
Ks(m/s) Sav(m) Theta-s Theta-i Sm(m) Schk(ponding ck)
```

IGR Input File (sampleBrOK0.igr)

```
2.2 .011 .001 .011 0
-----
SS(cm) Vn(s/cm1/3) H(cm) Vn2(s/m1/3) ICO(0 or 1)
```

ISD Input File (sampleBrOK0.isd)

1 .01 .000001 .434 Npart, Coarse, Ci(g/cm3), Por
.0023 2.6 Dp(cm), SG(g/cm3)

IRN Input File (sampleBrOK0.irn)

22 0.000017817 Nrain, rpeak (m/s)
0 .000017817
299.9 .000017817
599.8 .000017817
900 .000017817
1200 .000017817
1500 .000017817
1800 .000017817
2100 .000017817
2400 .000017817
2700 .000017817
3001 .000017817
4500 .000017817
6000 .000017817
6800 .000017817
7500 .000017817
8200 .000017817
9000 .000017817
10500 .000017817
11300 .000017817
13000 .000017817
13002 0
13603 0

IRO Input File (sampleBrOK0.iro)

.402 1 Swidth(m), Slength(m)
7 0.00005 nbcroff, bcropeak(m3/s)
0 .000005
3600 .000005
7200 .000005
10800 .000005
13000 .000005
13002 0
13603 0

IWQ Input File (sampleBrOK0.iwq)

```
3
'YuGao.xml' 'component_output_YuGao.xml' 'rs1'
1 water_column_p 103 0.045 2.08E-9 0
1 porewater_p 0
5 er .25E-6 h 0.000277 inf 0.0000118646 de 0.05 alpha .1475
0
depth 2.2 x_vel_ol 0 time_step 3600 area 0
```

Water Quality Project for Phosphorus Simulation in VFSSMOD

Project File (Bartow070706R2.prj)

ikw=inputs\Bartow070706R2.ikw
iso=inputs\Bartow070706R2.iso
igr=inputs\Bartow070706R2.igr
isd=inputs\Bartow070706R2.isd
irn=inputs\Bartow070706R2.irn
iro=inputs\Bartow070706R2.iro
iwq=inputs\Bartow070706R2.iwq
og1=output\Bartow070706R2.og1
og2=output\Bartow070706R2.og2
ohy=output\Bartow070706R2.ohy
osm=output\Bartow070706R2.osm
osp=output\Bartow070706R2.osp
owq=output\Bartow070706R2.owq

IKW Input File (Bartow070706R2.ikw)

Unit9, g8, u183-91
1.5
4.39 57 .5 .8 350 3 1 1
1
4.39 .048898 .018
1

ISO Input File (Bartow070706R2.iso)

0.00004074258667 0.10000000 0.450000 0.416463 0.000000 0.000000

Ks(m/s) Sav(m) Theta-s Theta-i Sm(m) Schk(ponding ck)

IGR Input File (Bartow070706R2.igr)

5.14 0.013 15.00 0.021 0

SS(cm) Vn(s/cm^{1/3}) H(cm) Vn2(s/m^{1/3}) ICO(0 or 1)

ISD Input File (Bartow070706R2.isd)

7 0.01 0.001 0.450 NPART, COARSE, Cl(g/cm³), POR
0.0022 2.59 DP(cm), SG(g/cm³)

IRN Input File (Bartow070706R2.irn)

6	2.7400e-05	
0.0000e+00		0.0000e+00
1.2000e+02		9.7900e-07
2.4000e+02		9.7900e-07
3.6000e+02		0.0000e+00
4.8000e+02		1.9600e-06
6.0000e+02		2.9400e-06
7.2000e+02		5.8800e-06
8.4000e+02		2.0600e-05
9.6000e+02		2.5500e-05
1.0800e+03		2.7400e-05
1.2000e+03		2.3500e-05
1.3200e+03		2.2500e-05
1.4400e+03		2.3500e-05
1.5600e+03		2.0600e-05
1.6800e+03		1.5700e-05
1.8000e+03		1.3700e-05
1.9200e+03		1.3700e-05
2.0400e+03		8.8200e-06
2.1600e+03		2.9400e-06
2.2800e+03		2.9400e-06
2.4000e+03		1.9600e-06
2.5200e+03		9.7900e-07
2.6400e+03		9.7900e-07
2.7600e+03		9.7900e-07
2.8800e+03		0.0000e+00
2.8220e+03		0.0000e+00

IWQ Input File (Bartow070706R2.iwq)

3
'Bartow.xml' 'component_output_Bartow.xml' 'rs1'
1 water_column_p 0.38 0.1 8.4E-10 0.0
0 porewater_p 0
7 Ka 6.91E-8 n -0.823 SSA 0.01066 pH 6.1 db 1.38 POR 0.47 CHK 1
0

IRO Input File (Bartow070706R2.iro)

3.3 14.4 Swidth(m), Slength(m)
33 0.000277155 nbcroff, bcropeak(m3/s)
960 0
1020 .0000233
1080 .0002231
1140 .00027716
1200 .00019946
1260 .00014808
1320 .00015425
1380 .00021714
1440 .00021262
1500 .00018775
1560 .00019885
1620 .00010019
1680 .0000352
1740 .0000277
1800 .0000233
1860 .0000217
1920 .0000137
1980 .0000124
2040 .0000108
2100 .0000106
2160 .0000101
2220 .00000941
2280 .00000877
2340 .00000827
2400 .00000752
2460 .00000703
2520 .00000655
2580 .00000318
2640 .00000139
2700 .000000929
2760 .000000692
2820 .000000349
2880 0

XML Input File used to Test RSE (Analytical Testing: Scenario I).

```
<?xml version="1.0" encoding="utf-8"?>
<wq version="0.1">
  <reaction_sets>
    <reaction_set name="rs1" full_name="Reaction Set Number 1">
      <coverage>
        <cell>all</cell>
        <segment>all</segment>
      </coverage>
      <stores>
        <store full_name="Surface Water" distribution="heterogeneous"
          location="element" section="gw" actuator="rsm_wm">
          <name>surface_water</name>
          <components>
            <variables>
              <variable type="mobile">
                <name full_name="Water Column P">water_column_p</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </variable>
              <variable type="mobile" section="o" >
                <name full_name="Ground Water P">gw_p</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </variable>
              <variable type="stable">
                <name full_name="Settled P">settled_p</name>
                <initial_distribution type="constant">
                  8.3
                </initial_distribution>
              </variable>
            </variables>
            <parameters>
              <parameter units="meter">
                <name>longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>molecular_diffusion</name>
                <initial_distribution type="constant">
                  0.00001
                </initial_distribution>
              </parameter>
              <parameter units="none">
                <name>surface_porosity</name>
                <initial_distribution type="constant">
                  1.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_transverse_dispersivity</name>

```

XML Input File used to Test RSE (scenario I)...continued

```

    <initial_distribution type="constant">
      10.0
    </initial_distribution>
  </parameter>
</parameter>
<parameter units="meter">
  <name>subsurface_molecular_diffusion</name>
  <initial_distribution type="constant">
    0.00001
  </initial_distribution>
</parameter>
<parameter units="none">
  <name>subsurface_porosity</name>
  <initial_distribution type="constant">
    1.0
  </initial_distribution>
</parameter>
<parameter units="none">
  <name>k_st</name>
  <initial_distribution type="constant">
    0.0
  </initial_distribution>
</parameter>
<parameter units="none">
  <name>k_rs</name>
  <initial_distribution type="constant">
    0.0
  </initial_distribution>
</parameter>
</parameters>
</components>
</store>
</stores>
<sw_gw_exchanges>
  <exchange>
    <surfacewater>water_column_p</surfacewater>
    <groundwater>gw_p</groundwater>
  </exchange>
</sw_gw_exchanges>
<equations>
  <equation>
    <lhs>water_column_p</lhs>
    <rhs>-k_st*water_column_p + k_rs*settled_p/depth</rhs>
  </equation>
  <equation>
    <lhs>settled_p</lhs>
    <rhs>depth*k_st*water_column_p - k_rs*settled_p</rhs>
  </equation>
</equations>
</reaction_set>
</reaction_sets>
</wq>

```

XML Input File used to Test TRT and TR-RSE for Linear Decay Kinetics.

```
<?xml version="1.0" encoding="utf-8"?>
<wq version="0.1">
  <reaction_sets>
    <reaction_set name="rs1" full_name="Reaction Set Number 1">
      <coverage>
        <cell>all</cell>
        <segment>all</segment>
      </coverage>
      <stores>
        <store full_name="Surface Water" distribution="heterogeneous"
          location="element" section="gw" actuator="rsm_wm">
          <name>surface_water</name>
          <components>
            <variables>
              <variable type="mobile">
                <name full_name="Water Column P">water_column_p</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </variable>
            </variables>
            <parameters>
              <parameter units="meter">
                <name>longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>molecular_diffusion</name>
                <initial_distribution type="constant">
                  0.00001
                </initial_distribution>
              </parameter>
              <parameter units="none">
                <name>surface_porosity</name>
                <initial_distribution type="constant">
                  1.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_molecular_diffusion</name>
                <initial_distribution type="constant">
                  0.00001
                </initial_distribution>
              </parameter>
              <parameter units="none">
                <name>subsurface_porosity</name>

```

XML Input File Used to Test TRT and TR-RSE for Linear Decay Kinetics..continued

```
<initial_distribution type="constant">
  1.0
</initial_distribution>
</parameter>
<parameter units="none">
  <name>k_st</name>
  <initial_distribution type="constant">
    0.0
  </initial_distribution>
</parameter>
<parameter units="none">
  <name>k_rs</name>
  <initial_distribution type="constant">
    0.0
  </initial_distribution>
</parameter>
</parameters>
</components>
</store>
</stores>
<equations>
  <equation>
    <lhs>water_column_p</lhs>
    <rhs>k_st*water_column_p</rhs>
  </equation>
</equations>
</reaction_set>
</reaction_sets>
</wq>
```

YuGao.xml Water Quality Input File.

```
<?xml version="1.0" encoding="utf-8"?>
<wq version="0.1">
  <reaction_sets>
    <reaction_set name="rs1" full_name="Reaction Set Number 1">
      <coverage>
        <cell>all</cell>
        <segment>all</segment>
      </coverage>
      <stores>
        <store full_name="Surface Water" distribution="heterogeneous"
          location="element" section="gw" actuator="rsm_wm">
          <name>surface_water</name>
          <components>
            <variables>
              <variable type="mobile">
                <name full_name="Water Column P">water_column_p</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </variable>
              <variable type="stable">
                <name full_name="Porewater P">porewater_p</name>
                <initial_distribution type="constant">
                  8.3
                </initial_distribution>
              </variable>
            </variables>
            <parameters>
              <parameter units="meter">
                <name>longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>molecular_diffusion</name>
                <initial_distribution type="constant">
                  0.00001
                </initial_distribution>
              </parameter>
              <parameter units="none">
                <name>surface_porosity</name>
                <initial_distribution type="constant">
                  1.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_molecular_diffusion</name>

```

YuGao.xml Water Quality Input File...continued

```

    <initial_distribution type="constant">
      0.00001
    </initial_distribution>
  </parameter>
</parameter>
<parameter units="none">
  <name>subsurface_porosity</name>
  <initial_distribution type="constant">
    1.0
  </initial_distribution>
</parameter>
<parameter units="none">
  <name>er</name>
  <initial_distribution type="constant">
    0.0
  </initial_distribution>
</parameter>
<parameter units="none">
  <name>inf</name>
  <initial_distribution type="constant">
    0.0
  </initial_distribution>
</parameter>
  <parameter units="none">
    <name>h</name>
    <initial_distribution type="constant">
      0.0
    </initial_distribution>
  </parameter>
  <parameter units="none">
    <name>de</name>
    <initial_distribution type="constant">
      0.0
    </initial_distribution>
  </parameter>
  <parameter units="none">
    <name>alpha</name>
    <initial_distribution type="constant">
      0.0
    </initial_distribution>
  </parameter>
</parameters>
</components>
</store>
</stores>
<equations>
  <equation>
    <lhs>water_column_p</lhs>
    <rhs>er*(porewater_p-alpha*water_column_p)/h</rhs>
  </equation>
  <equation>
    <lhs>porewater_p</lhs>
    <rhs>(inf+er)*(alpha*water_column_p-porewater_p)/de</rhs>
  </equation>
</equations>
</reaction_set>
</reaction_sets>
</wq>

```

Bartow.xml Water Quality Input File.

```
<?xml version="1.0" encoding="utf-8"?>
<wq version="0.1">
  <reaction_sets>
    <reaction_set name="rs1" full_name="Reaction Set Number 1">
      <coverage>
        <cell>all</cell>
        <segment>all</segment>
      </coverage>
      <stores>
        <store full_name="Surface Water" distribution="heterogeneous"
          location="element" section="gw" actuator="rsm_wm">
          <name>surface_water</name>
          <components>
            <variables>
              <variable type="mobile">
                <name full_name="Water Column P">water_column_p</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </variable>
            </variables>
            <parameters>
              <parameter units="meter">
                <name>longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>molecular_diffusion</name>
                <initial_distribution type="constant">
                  0.00001
                </initial_distribution>
              </parameter>
              <parameter units="none">
                <name>surface_porosity</name>
                <initial_distribution type="constant">
                  1.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_longitudinal_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_transverse_dispersivity</name>
                <initial_distribution type="constant">
                  10.0
                </initial_distribution>
              </parameter>
              <parameter units="meter">
                <name>subsurface_molecular_diffusion</name>
                <initial_distribution type="constant">
                  0.00001
                </initial_distribution>
              </parameter>
              <parameter units="none">
                <name>subsurface_porosity</name>

```

Bartow.xml water quality input file...continued

```
</initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>TSED</name>
<initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>FSED</name>
<initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>CSED</name>
<initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>SEDFVS</name>
<initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>FPI</name>
<initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>HRO</name>
<initial_distribution type="constant">
1.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>Ka</name>
<initial_distribution type="constant">
0.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>n</name>
<initial_distribution type="constant">
0.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>SSA</name>
<initial_distribution type="constant">
0.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>pH</name>
<initial_distribution type="constant">
0.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>db</name>
```

Bartow.xml water quality input file...continued

```
<initial_distribution type="constant">
0.0
</initial_distribution>
</parameter>
<parameter units="none">
<name>POR</name>
<initial_distribution type="constant">
0.0
</initial_distribution>
</parameters>
</components>
</store>
</stores>
<equations>
<equation>
<lhs>water_column_p</lhs>
<rhs>31*Ka*(10^(-pH))^n*SSA*db/POR</rhs>
</equation>
</equations>
</reaction_set>
</reaction_sets>
</wq>
```

APPENDIX B. FIELD SCALE EXPERIMENTAL DATA

A summary of the experimental data is presented in this appendix. Results are presented as Tables for the hydrological and water quality sets of data. It is important to point out that only years 2007 and 2008 are presented. For more details on data from 2005 to 2006, please review Kuo (2007)

Hydrological data are presented first, followed by data of loads of sediments, phosphates and particulate phosphorus.

Table B-1. Summary of rain and runoff data for the river experimental site (A) during 2007.

Event Date	Rain m	Total Time min	i30 mm /h	A-Source-1			A-Source-2			A-Source-3			A-Source-4			A-VFS-1			A-VFS-2			A-VFS-3			A-VFS-4		
				Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi									
01/28/07	1.8	29	3.6	0.000	0.000	0.064	0.000	0.000	0.048	0.000	0.000	0.062	0.000	0.000	0.051	0.000	0.000	0.082	0.000	0.000	0.172	0.000	0.000	0.347	0.000	0.000	0.159
02/02/07*	34	70	52.2	0.326	1.088	0.041	0.422	1.2843	0.035	0.506	1.157	0.041	0.190	0.570	0.030	0.008	0.130	0.063	0.044	0.064	0.108	0.109	0.420	0.041	0.075	0.152	0.115
02/13/07	6.3	37	11.8	0.000	0.000	0.038	0.000	0.000	0.036	0.000	0.000	0.039	0.000	0.000	0.031	0.000	0.000	0.055	0.000	0.000	0.092	0.000	0.000	0.197	0.000	0.000	0.109
04/10/07	15.6	82	21.2	0.014	0.097	0.047	0.016	0.098	0.039	0.412	0.282	0.046	0.009	0.057	0.037	0.000	0.000	0.032	0.000	0.000	0.128	0.000	0.000	0.162	0.000	0.000	0.079
04/15/07*	18.3	33	36.6	0.147	0.810	0.037	0.181	0.813	0.031	0.219	0.859	0.036	0.114	0.407	0.026	0.000	0.000	X	0.008	0.017	0.114	0.005	0.026	0.037	0.052	0.226	0.066
05/04/07	14	69	23	0.005	0.009	0.018	0.004	0.015	0.016	0.010	0.057	0.017	X	X	0.011	X	X	0.012	0.000	0.000	0.047	0.000	0.000	0.124	0.000	0.000	0.013
05/06/07*	20.1	20	40.2	0.058	0.264	0.044	0.105	0.417	0.037	0.176	0.700	0.041	0.056	0.237	0.032	X	X	0.023	0.011	0.018	0.112	X	X	0.119	0.009	0.010	0.067
05/16/07	7.4	51	10.6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/30/07	14.5	67	18.4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/01/07	13.4	33	26.6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/02/07	16.5	49	31.8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/06/07	9	59	17.4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/10/07	6.6	51	9.2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/13/07	17.9	39	32.2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/31/07	4	40	5.6	0.000	0.000	0.038	0.000	0.000	0.036	0.000	0.000	0.039	0.000	0.000	0.031	0.000	0.000	0.055	0.000	0.000	0.092	0.000	0.000	0.197	0.000	0.000	0.109
08/02/07	4.1	27	8.2	0.000	0.000	0.038	0.000	0.000	0.036	0.000	0.000	0.039	0.000	0.000	0.031	0.000	0.000	0.055	0.000	0.000	0.092	0.000	0.000	0.197	0.000	0.000	0.109
08/06/07	3.1	33	3.1	0.000	0.000	0.038	0.000	0.000	0.036	0.000	0.000	0.039	0.000	0.000	0.031	0.000	0.000	0.055	0.000	0.000	0.092	0.000	0.000	0.197	0.000	0.000	0.109
08/11/07*	12.3	20	24.6	X	X	0.024	0.014	0.071	0.014	0.015	0.072	0.023	0.005	0.012	0.018	0.051	0.174	0.050	0.014	0.034	0.014	0.022	0.081	0.024	0.125	0.391	0.017
08/31/07	36.4	60	56	0.151	0.233	0.036	0.096	0.401	0.023	0.098	0.431	0.032	0.018	0.104	0.027	0.139	0.228	0.064	0.051	0.094	0.023	0.002	0.152	0.035	0.124	0.219	0.079
09/01/07	14.7	31	29.2	0.065	0.123	0.094	0.008	0.016	0.086	0.035	0.088	0.087	0.000	0.000	0.066	0.000	0.000	0.076	0.017	0.029	0.118	0.000	0.000	0.084	0.003	0.006	0.182
09/04/07	2.5	44	4.8	0.000	0.000	0.051	0.000	0.000	0.039	0.000	0.000	0.047	0.000	0.000	0.038	0.000	0.000	0.029	0.000	0.000	0.067	0.000	0.000	0.006	0.000	0.000	0.119
09/07/07*	8.3	23	16.6	0.014	0.021	0.039	0.000	0.000	0.027	0.000	0.000	0.036	0.000	0.000	0.028	0.000	0.000	0.011	0.013	0.027	0.033	0.000	0.000	0.010	0.005	0.006	0.084
09/08/07	2.3	32	4.6	0.000	0.000	0.061	0.000	0.000	0.045	0.000	0.000	0.049	0.000	0.000	0.047	0.000	0.000	0.055	0.000	0.000	0.092	0.000	0.000	0.035	0.000	0.000	0.136
09/12/07*	41.5	122	38.8	0.094	0.138	0.044	0.073	0.313	0.030	0.058	0.316	0.038	0.017	0.092	0.030	0.000	0.000	0.025	0.095	0.068	0.047	0.000	0.000	0.015	0.003	0.009	0.101
10/05/07*	40	309	43.4	0.021	0.018	0.043	0.049	0.122	0.031	0.007	0.036	0.041	0.000	0.000	0.037	0.000	0.000	0.046	0.026	0.029	0.067	0.000	0.000	0.043	0.060	0.051	0.137
10/06/07	1.1	83	0.7	0.000	0.000	0.054	0.000	0.000	0.045	0.000	0.000	0.051	0.000	0.000	0.042	0.000	0.000	0.059	0.000	0.000	0.099	0.000	0.000	0.039	0.000	0.000	0.146
10/07/07	14.2	107	16.2	0.008	0.008	0.055	0.011	0.010	0.039	0.015	0.010	0.048	0.000	0.000	0.038	0.000	0.000	0.050	0.008	0.009	0.086	0.000	0.000	0.053	0.066	0.048	0.139
10/23/07*	11.6	27	23.2	0.012	0.010	0.029	0.014	0.021	0.030	0.007	0.489	0.033	0.000	0.000	0.029	0.000	0.000	0.004	0.009	0.014	0.038	0.000	0.000	0.030	0.047	0.050	0.072
12/14/07	7.3	64	13.8	0.000	0.000	0.021	0.000	0.000	0.014	0.000	0.000	0.020	0.000	0.000	0.017	0.000	0.000	X	0.000	0.000	0.002	0.000	0.000	X	0.000	0.000	0.022
12/16/07	0.7	29	1.4	0.000	0.000	0.067	0.000	0.000	0.052	0.000	0.000	0.039	0.000	0.000	0.062	0.000	0.000	0.007	0.000	0.000	0.079	0.000	0.000	0.032	0.000	0.000	0.086
12/21/07	2.4	66	2.4	0.000	0.000	0.041	0.000	0.000	0.029	0.000	0.000	0.031	0.000	0.000	0.035	0.000	0.000	X	0.000	0.000	0.061	0.000	0.000	0.002	0.000	0.000	0.079
12/30/07	5.7	43	9	0.000	0.000	0.053	0.000	0.000	0.037	0.000	0.000	0.030	0.000	0.000	0.040	0.000	0.000	0.010	0.000	0.000	0.117	0.000	0.000	0.023	0.000	0.000	0.114

*: Samples collected automatically for chemical analysis

X: Under maintenance or equipment failure

Table B-2. Summary of rain and runoff data for the river experimental site (A) during 2008.

Event Date	Rain mm	Total Time min	130 mm/ h	A-Source-1			A-Source-2			A-Source-3			A-Source-4			A-VFS-1			A-VFS-2			A-VFS-3			A-VFS-4		
				Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi									
01/01/08	1.1	106	1	0.000	0.000	0.039	0.000	0.000	0.037	0.000	0.000	0.039	0.000	0.000	0.030	0.000	0.000	0.054	0.000	0.000	0.092	0.000	0.000	0.197	0.000	0.000	0.108
01/22/08	0.8	67	1	0.000	0.000	0.026	0.000	0.000	0.024	0.000	0.000	0.027	0.000	0.000	0.020	0.000	0.000	0.032	0.000	0.000	0.051	0.000	0.000	0.320	0.000	0.000	0.051
01/25/08	23.2	631	5	0.000	0.000	0.055	0.000	0.000	0.043	0.000	0.000	0.055	0.000	0.000	0.045	0.000	0.000	0.068	0.000	0.000	0.148	0.000	0.000	0.234	0.000	0.000	0.143
01/28/08	9.5	190	6	0.000	0.000	0.052	0.000	0.000	0.043	0.000	0.000	0.052	0.000	0.000	0.041	0.000	0.000	0.074	0.000	0.000	0.143	0.000	0.000	0.228	0.000	0.000	0.140
02/08/08	3.7	44	7.2	0.000	0.000	0.032	0.000	0.000	0.022	0.000	0.000	0.028	0.000	0.000	0.026	0.000	0.000	X	0.000	0.000	0.003	0.000	0.000	0.068	0.000	0.000	0.052
02/12/08	6.9	56	11.8	0.000	0.000	0.036	0.000	0.000	0.027	0.000	0.000	0.034	0.000	0.000	0.034	0.000	0.000	0.001	0.000	0.000	0.016	0.000	0.000	0.087	0.000	0.000	0.061
02/21/08	4.1	37	8.2	0.000	0.000	0.052	0.000	0.000	0.035	0.000	0.000	0.032	0.000	0.000	0.032	0.000	0.000	X	0.000	0.000	0.070	0.000	0.000	0.126	0.000	0.000	0.089
02/23/08*	20.3	152	25.4	0.012	0.010	0.042	0.022	0.126	0.044	0.083	0.113	0.035	0.007	0.009	0.034	0.000	0.000	X	0.022	0.031	0.039	0.000	0.000	0.097	0.000	0.000	0.077
03/07/08	3.9	80	3.6	0.000	0.000	0.085	0.000	0.000	0.066	0.000	0.000	0.061	0.000	0.000	0.068	0.000	0.000	X	0.000	0.000	0.114	0.000	0.000	0.156	0.000	0.000	0.145
03/08/08	1.5	60	1.2	0.000	0.000	0.075	0.000	0.000	0.058	0.000	0.000	0.058	0.000	0.000	0.061	0.000	0.000	0.001	0.000	0.000	0.096	0.000	0.000	0.145	0.000	0.000	0.131
03/11/08	1.8	35	3.6	0.000	0.000	0.049	0.000	0.000	0.033	0.000	0.000	0.038	0.000	0.000	0.038	0.000	0.000	0.001	0.000	0.000	0.064	0.000	0.000	0.113	0.000	0.000	0.096
03/12/08	7.3	32	14.6	0.007	0.027	0.057	0.061	0.079	0.037	0.003	0.011	0.038	0.000	0.000	0.043	0.000	0.000	0.001	0.016	0.033	0.076	0.000	0.000	0.118	0.004	0.011	0.108
03/14/08	18.8	258	15.6	0.000	0.000	0.049	0.000	0.000	0.035	0.000	0.000	0.044	0.000	0.000	0.039	0.000	0.000	X	0.000	0.000	0.073	0.000	0.000	0.117	0.000	0.000	0.099
03/20/08	5	62	5.4	0.000	0.000	0.052	0.000	0.000	0.040	0.000	0.000	0.042	0.000	0.000	0.040	0.000	0.000	X	0.000	0.000	0.084	0.000	0.000	0.113	0.000	0.000	0.109
03/22/08	6.9	296	2.6	0.000	0.000	0.046	0.000	0.000	0.033	0.000	0.000	0.039	0.000	0.000	0.037	0.000	0.000	X	0.000	0.000	0.078	0.000	0.000	0.107	0.000	0.000	0.096
04/02/08	8.4	341	2.8	0.000	0.000	0.047	0.000	0.000	0.034	0.000	0.000	0.041	0.000	0.000	0.038	0.000	0.000	X	0.000	0.000	0.054	0.000	0.000	0.105	0.000	0.000	0.087
04/07/08	0.9	61	1.2	0.000	0.000	0.047	0.000	0.000	0.034	0.000	0.000	0.041	0.000	0.000	0.038	0.000	0.000	X	0.000	0.000	0.054	0.000	0.000	0.105	0.000	0.000	0.087

*: Samples collected automatically for chemical analysis

X: Under maintenance or equipment failure

Table B-3. Summary of rain and runoff data for the hill experimental site (B) during 2007.

Event Date	Rain mm	Total Time min	I30 mm/h	B-Source-1			B-Source-2			B-Source-3			B-Source-4			B-VFS-1			B-VFS-2			B-VFS-3			B-VFS-4		
				Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi	Q, m3	Qp, L/s	θi									
01/28/07	5.2	45	7.6	0.000	0.000	0.381	0.000	0.000	0.272	0.000	0.000	0.186	0.000	0.000	0.182	0.000	0.000	0.074	0.000	0.000	0.220	0.000	0.000	0.233	0.000	0.000	0.091
02/02/07	36.322	221	15.748+	4.314	6.921	0.373	X	X	0.253	1.572	3.930	0.174	0.385	1.281	0.162	2.238	3.991	X	0.986	3.148	0.215	0.007	0.031	0.225	0.022	0.026	0.097
02/27/07	0.8	38	1.6	0.000	0.000	0.370	0.000	0.000	0.241	0.000	0.000	0.172	0.000	0.000	0.162	0.000	0.000	0.090	0.000	0.000	0.201	0.000	0.000	0.218	0.000	0.000	0.085
03/03/07	1.1	72	1.6	0.000	0.000	0.369	0.000	0.000	0.240	0.000	0.000	0.169	0.000	0.000	0.170	0.000	0.000	0.071	0.000	0.000	0.194	0.000	0.000	0.215	0.000	0.000	0.081
03/16/07	1.9	38	3	0.000	0.000	0.353	0.000	0.000	0.229	0.000	0.000	0.158	0.000	0.000	0.138	0.000	0.000	0.080	0.000	0.000	0.010	0.000	0.000	0.178	0.000	0.000	0.018
04/05/07	1.1	58	1	0.000	0.000	0.337	0.000	0.000	0.223	0.000	0.000	0.151	0.000	0.000	0.156	0.000	0.000	X									
04/09/07	2.6	70	4.8	0.000	0.000	0.328	0.000	0.000	0.220	0.000	0.000	0.149	0.000	0.000	0.139	0.000	0.000	0.088	0.000	0.000	0.014	0.000	0.000	0.071	0.000	0.000	X
04/10/07	6	148	5	0.000	0.000	0.339	0.000	0.000	0.223	0.000	0.000	0.151	0.000	0.000	0.147	0.000	0.000	X	0.000	0.000	0.008	0.000	0.000	X	0.000	0.000	0.014
04/11/07	6.9	48	6	0.000	0.000	0.400	0.000	0.000	0.285	0.000	0.000	0.202	0.000	0.000	0.220	0.000	0.000	X	0.000	0.000	0.122	0.000	0.000	X	0.000	0.000	0.053
04/15/07*	5.1	56	9.2	1.348	0.175	0.375	1.537	0.139	0.248	1.092	0.092	0.178	0.739	0.070	0.174	0.784	0.043	X	0.666	0.069	0.097	0.002	0.000	0.069	0.048	0.008	0.046
05/04/07	18.9	121	27.8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/06/07	27.8	45	25.6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/07/07	16.2	92	19.2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/13/07	8.7	131	11.8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/14/07	1.4	44	2.4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/16/07	6.7	71	7.4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/17/07	1.4	25	2.8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
05/25/07	1.27	26	2.54+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/01/07	11.176	111	9.144+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/02/07	5.08	121	4.064+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/06/07	3.81	96	7.62+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/07/07	1.27	26	2.54+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/13/07	1.27	41	2.032+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/22/07	8.636	46	16.764+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
06/30/07	12.192	101	13.208+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/01/07	16.002	106	15.748+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/02/07	12.7	46	24.892+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/06/07	4.318	26	8.636+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/09/07	1.27	31	2.54+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/10/07	9.144	46	17.272+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/13/07	11.43	71	20.828+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/14/07	2.032	41	3.556+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/15/07	5.334	56	7.62+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/19/07	2.286	31	4.572+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/21/07	18.288	436	5.08+	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
07/22/07	5.334	76	4.572+	0.000	0.000	X	0.000	0.000	0.083	0.000	0.000	0.084	0.000	0.000	0.044	0.000	0.000	0.187	0.000	0.000	0.139	0.000	0.000	0.295	0.000	0.000	0.098
07/25/07	4.572	31	9.144+	0.000	0.000	X	0.000	0.000	0.086	0.000	0.000	0.087	0.000	0.000	0.054	0.000	0.000	0.227	0.000	0.000	0.124	0.000	0.000	0.105	0.000	0.000	0.094
07/31/07	7.112	191	5.08+	0.000	0.000	X	0.000	0.000	X	0.000	0.000	X	0.000	0.000	X	0.000	0.000	X									
08/01/07	4.3	28	8.6	0.000	0.000	X	0.000	0.000	X	0.000	0.000	X	0.000	0.000	X	0.000	0.000	X									

Table B-3...continued

08/24/07*	25.57	140	17.18+	0.509	1.692	0.236	X	X	0.041	0.166	0.474	0.068	0.175	0.469	0.047	0.008	0.026	0.09	0.125	0.052	0.15	0.000	0.000	0.011	0.013	0.084	M
08/31/07*	37.3	70	56.8+	6.561	10.749	0.036	3.550	13.011	0.026	5.206	13.019	0.032	1.951	7.150	0.027	0.262	0.641	M	0.330	0.822	0.023	0.010	0.013	M	0.001	0.011	0.079
09/01/07*	18.94	80	34.96+	0.405	1.387	0.349	0.192	0.594	0.155	0.124	0.515	0.2	0.056	0.207	0.155	0.000	0.000	0.06	0.000	0.000	0.15	0.003	0.003	0.073	0.000	0.000	0.062
09/12/07*	22.26	107	18.84+	0.920	9.117	X	X	X	0.08	0.115	0.244	0.169	0.030	0.015	0.1	0.000	0.000	0.029	0.000	0.000	0.109	0.000	0.000	0.066	0.000	0.000	0.062
10/02/07	1.016	41	2.032+	0.000	0.000	0.256	0.000	0.000	0.09	0.000	0.000	0.195	0.000	0.000	0.137	0.000	0.000	0.075	0.000	0.000	0.077	0.000	0.000	0.02	0.000	0.000	0.299
10/03/07	1.016	56	1.524+	0.000	0.000	0.174	0.000	0.000	0.085	0.000	0.000	0.189	0.000	0.000	0.127	0.000	0.000	0.072	0.000	0.000	0.072	0.000	0.000	0.022	0.000	0.000	0.124
10/05/07*	25.908	321	25.4+	3.437	4.669	0.383	22.649	13.579	0.081	11.940	12.886	0.18	4.480	7.015	0.126	1.457	3.131	0.065	X	X	0.069	X	X	0.225	X	X	0.346
10/06/07	0.508	31	1.016+	0.000	0.000	0.374	0.000	0.000	0.119	0.000	0.000	0.212	0.000	0.000	0.165	0.000	0.000	0.100	0.000	0.000	0.096	0.000	0.000	0.012	0.000	0.000	0.476
10/19/07	4.572	31	9.144+	0.000	0.000	0.277	0.000	0.000	0.076	0.000	0.000	0.167	0.000	0.000	0.097	0.000	0.000	0.070	0.000	0.000	0.032	0.000	0.000	X	0.000	0.000	0.414
10/20/07	2.032	41	3.556+	0.000	0.000	X	0.000	0.000	0.087	0.000	0.000	0.179	0.000	0.000	0.113	0.000	0.000	0.078	0.000	0.000	0.052	0.000	0.000	X	0.000	0.000	0.43
10/23/07	14.478	61	26.924+	0.094	0.431	0.39	0.020	0.026	0.086	0.000	0.000	0.169	0.086	0.144	0.105	0.000	0.000	0.074	0.000	0.000	0.042	0.000	0.000	X	0.000	0.000	0.43
10/28/07	1.524	31	3.048+	0.000	0.000	0.378	0.000	0.000	0.092	0.000	0.000	0.183	0.000	0.000	0.123	0.000	0.000	0.094	0.000	0.000	0.083	0.000	0.000	0.004	0.000	0.000	0.422
10/30/07	1.27	36	2.54+	0.000	0.000	0.383	0.000	0.000	0.103	0.000	0.000	0.204	0.000	0.000	0.151	0.000	0.000	0.112	0.000	0.000	0.102	0.000	0.000	0.08	0.000	0.000	0.428
12/14/07	6.3	62	5.8	0.000	0.000	0.373	0.000	0.000	0.038	0.000	0.000	0.07	0.000	0.000	X	0.000	0.000	0.025	0.000	0.000	0.008	0.000	0.000	X	0.000	0.000	0.43
12/16/07	2	36	4	0.000	0.000	0.342	0.000	0.000	0.063	0.000	0.000	0.131	0.000	0.000	X	0.000	0.000	0.063	0.000	0.000	0.078	0.000	0.000	0.031	0.000	0.000	0.438
12/21/07	2.5	56	2.8	0.000	0.000	0.375	0.000	0.000	0.057	0.000	0.000	0.116	0.000	0.000	X	0.000	0.000	0.068	0.000	0.000	0.066	0.000	0.000	0.298	0.000	0.000	0.426

*: Samples collected automatically for chemical analysis

X: Under maintenance or equipment failure

Table B-4. Summary of rain and runoff data for the hill experimental site (B) during 2008.

Event	Rain	Total	I30	B-Source-1			B-Source-2			B-Source-3			B-Source-4			B-VFS-1			B-VFS-2			B-VFS-3			B-VFS-4		
Date	mm	min	mm/h	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i	Q _i m ³	Q _p L/s	θ _i
01/22/08	0.9	69	1.4	0.000	0.000	0.350	0.000	0.000	0.167	0.000	0.000	0.113	0.000	0.000	0.111	0.000	0.000	X	0.000	0.000	0.122	0.000	0.000	0.184	0.000	0.000	0.047
01/27/08	0.4	29	0.8	0.000	0.000	X	0.000	0.000	0.273	0.000	0.000	0.186	0.000	0.000	0.180	0.000	0.000	X	0.000	0.000	0.220	0.000	0.000	0.231	0.000	0.000	0.090
01/28/08	11	262	8.2	0.000	0.000	X	0.000	0.000	0.304	0.000	0.000	0.211	0.000	0.000	0.209	0.000	0.000	X	0.000	0.000	0.243	0.000	0.000	0.247	0.000	0.000	0.103
02/08/08	0.9	110	0.8	0.000	0.000	0.357	0.000	0.000	0.083	0.000	0.000	0.177	0.000	0.000	X	0.000	0.000	0.057	0.000	0.000	0.057	0.000	0.000	0.276	0.000	0.000	0.413
02/12/08	7.1	47	13	0.000	0.000	X	0.000	0.000	0.079	0.000	0.000	0.165	0.000	0.000	X	0.000	0.000	0.047	0.000	0.000	0.058	0.000	0.000	0.019	0.000	0.000	0.426
02/23/08*	15.6	293	22.8	0.268	0.982	0.317	0.034	0.075	0.083	0.113	0.504	0.166	0.073	0.216	X	0.002	0.005	0.050	0.000	0.000	0.094	0.000	0.000	0.332	0.000	0.000	0.430
03/06/08	20.9	317	15.2	0.013	0.017	0.032	0.007	0.028	0.059	0.000	0.000	0.142	0.013	0.030	X	0.002	0.004	0.047	0.004	0.016	0.112	0.000	0.000	0.114	0.000	0.000	0.125
03/07/08	1	29	2	0.000	0.000	0.196	0.000	0.000	0.122	0.000	0.000	0.198	0.000	0.000	X	0.000	0.000	0.094	0.000	0.000	0.212	0.000	0.000	0.256	0.000	0.000	0.212
03/08/08	4.5	147	3.2	0.000	0.000	0.073	0.000	0.000	0.157	0.000	0.000	0.260	0.000	0.000	0.001	0.000	0.000	0.163	0.000	0.000	0.138	0.000	0.000	0.172	0.000	0.000	0.170
03/11/08	3.8	58	6	0.000	0.000	0.136	0.000	0.000	0.119	0.000	0.000	0.205	0.000	0.000	X	0.000	0.000	0.125	0.000	0.000	0.125	0.000	0.000	0.020	0.000	0.000	0.148
03/12/08	3.5	337	1.8	0.000	0.000	0.107	0.000	0.000	0.131	0.000	0.000	0.230	0.000	0.000	X	0.000	0.000	0.144	0.000	0.000	0.139	0.000	0.000	0.133	0.000	0.000	0.171
03/20/08	0.8	150	0.8	0.000	0.000	0.144	0.000	0.000	0.108	0.000	0.000	0.194	0.000	0.000	0.061	0.000	0.000	0.100	0.000	0.000	0.129	0.000	0.000	0.004	0.000	0.000	0.172
03/23/08	8.4	674	1.4	0.000	0.000	0.156	0.000	0.000	0.142	0.000	0.000	0.233	0.000	0.000	0.092	0.000	0.000	0.138	0.000	0.000	0.149	0.000	0.000	0.041	0.000	0.000	0.201
04/02/08	34.8	852	8.2	0.000	0.000	0.007	0.000	0.000	0.140	0.000	0.000	0.234	0.000	0.000	0.085	0.000	0.000	0.153	0.000	0.000	0.149	0.000	0.000	X	0.000	0.000	0.200
04/03/08	0.8	47	1.8	0.000	0.000	0.203	0.000	0.000	0.139	0.000	0.000	0.232	0.000	0.000	0.086	0.000	0.000	0.153	0.000	0.000	0.149	0.000	0.000	X	0.000	0.000	0.199
04/07/08	0.9	61	1	0.000	0.000	0.151	0.000	0.000	0.163	0.000	0.000	0.188	0.000	0.000	0.126	0.000	0.000	0.203	0.000	0.000	0.165	0.000	0.000	X	0.000	0.000	0.206

*: Samples collected automatically for chemical analysis

X: Under maintenance or equipment failure

Table B-5. Summary of loads of sediment and phosphorus for the river experimental site (A) during 2007 and 2008.

Site A (River)	A –Source 1			A – Source 2			A –Source 3			A –Source 4			A - VFS 1			A - VFS 2			A - VFS 3			A - VFS 4		
	LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g		
Date	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP
02/02/07	X	X	X	21.392	0.144	-	16.862	1.124	0.209	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
04/15/07	X	X	X	30.335	2.790	0.101	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	1.085	0.057	0.030
05/06/07	X	X	X	-	0.459	0.425	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
08/11/07	X	X	X	-	0.029	0.014	-	0.093	0.019	X	X	X	+	+	+	+	+	+	1.408	0.112	0.086	+	+	+
09/07/07	X	X	X	+	+	+	+	+	+	X	X	X	+	+	+	-	0.017	0.007	+	+	+	+	+	+
09/12/07	X	X	X	-	0.083	0.021	1.833	0.184	0.029	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
10/05/07	X	X	X	1.005	0.131	0.013	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
10/23/07	X	X	X	-	0.013	0.004	-	0.113	0.010	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
02/23/08	X	X	X	-	0.015	0.011	12.536	0.101	0.039	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+

Sed: Sediments

TP: Total Phosphorus

DP: Dissolved Phosphorus

+: No water sample collected

-: Not enough water in collection bottles for chemical analysis

X: No automatic sample collector in this site

Table B-6. Summary of loads of sediment and phosphorus for the hill experimental site (B) during 2007 and 2008.

Site B (Hill)	Source Area 1			Source Area 2			Source Area 3			Source Area 4			VFS 1			VFS 2			VFS 3			VFS 4		
	LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g			LOAD, g		
Date	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP	Sed	TP	DP
04/15/07	X	X	X	1692.7	147.2	1.9	-	-	-	X	X	X	+	+	+	+	+	+	+	+	+	7.45	0.86	0.10
08/24/07	X	X	X	+	+	+	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
08/31/07	X	X	X	+	+	+	167.7	7.6	0.15	X	X	X	11.47	0.89	0.19	+	+	+	5.69	0.82	0.13	+	+	+
09/01/07	X	X	X	87.5	-	-	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
09/12/07	X	X	X	+	+	+	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
10/05/07	X	X	X	5858.0	296.7	12.4	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+
02/23/08	X	X	X	11.02	0.12	0.02	+	+	+	X	X	X	+	+	+	+	+	+	+	+	+	+	+	+

Sed: Sediments

TP: Total Phosphorus

DP: Dissolved Phosphorus

+: No water sample collected

-: Not enough water in collection bottles for chemical analysis

X: No automatic sample collector in this site

Table B-7. Summary of rainfall-runoff events recorded at sites River (A) and Hill (B) for the period January 2007 to April 2008.

Total events with rain									Only events that produced runoff							
Site	n	Rainfall duration, min	Total rain, mm	i30+	N	Rainfall duration, min	Total rainfall, mm	i30+	Plot*	N	V (m ³ /ha)	Qp (L/s)	qi, %	Sediment (kg/ha)	TP (kg/ha)	DP (kg/ha)
River (A)	51	20-631 (9.1,2.9)#	0.7-62.8 (5.4,2.1)#	0.7-62.8 (5.4,2.1)#	15	20-309 (6.1,2.3)#	7.3-41.5 (0.7,0.9)#	14.6-56.0 (-0.6,0.6)#	Source Area A	15	0-106.6	0-1.3	0.01-0.09	6.38	0.59	0.09
									A6	13	0-72.5	0-0.4	0.01-0.16	0.74	0.06	0.05
									A4	10	0-92.2	0-1.1	0.01-0.18	0.80	0.04	0.02
Hill (B)	79	25-852 (12,3.2)#	0.8-56.8 (5.51,2.1)#	0.8-56.8 (5.51,2.1)@	10@	56-321 (-1.7,0.5)#	5.1-37.3 (0.03,0.07)#	9.2-56.8 (3.5,1.7)@	Source Area B	10	0-1715	0-13	0.02-0.38	443.80	22.48	0.94
									B-13	8	0-506	0-4	0.1-0.3	2.59	0.20	0.04
									B7	8	0-439	0-3.1	0.01-0.40	3.32	0.38	0.04

n: Number of events.

N: Number of events with runoff only

* A6: Include VFS plots 1 and 3 (5.8m long) from River site. A4: include plots VFS-2 and VFS-4 (4.1 m long) in the River site; B13: include plots VFS1 and VFS3 (13.4 m long) in the Hill site; B7: includes plots VFS-2 and VFS-2 (6.8 m long) in Hill site.

+i₃₀: maximum 30-minute rainfall intensity

#: Values in parenthesis are (kurtosis, skewness).

@: adapted from various sources

APPENDIX C PROGRAM SOURCE CODE

This appendix contains the VFSSMOD-W fortran source code files that were modified for coupling RSE to VFSSMOD-W. Only those files that were modified are presented here, in addition to the corresponding fortran files of RSE.

The full code for VFSSMOD-W can be downloaded from:

<http://abe.ufl.edu/carpena/vfssmod/index.shtml> (accessed on July, 2010).


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C time step by the extension of the Green-Ampt method as proposed by C
C Mein& Larson, (1967) and Chu (1975), C
C
C The overland flow solution is linked to a submodel to calculate C
C sediment transport on a grass filter. The information from the C
C submodel is used to assemble the vector {b} during the procedure C
C described above. C
C The sediment filtration is based on the method proposed by: C
C
C 1. Tollner et al. (1976). "Suspended sediment filtration capacity of C
C simulated vegetation". Trans. ASAE. 19(4):698-682. C
C 2. Tollner et al. (1977). "Sediment deposition patterns in simulated C
C grass filters". Trans. ASAE. 20(5):940-944. C
C 3. Barfield et. al (1979)"Filtration of sediment by simulated vegetation C
C I. Trans. ASAE, 22(3):540-548. C
C 4. Hayes et. al (1979)"Filtration of sediment by simulated vegetationII" C
C Trans. ASAE, 22(5):1063-1067 C
C 5. Hayes et. al (1984)"Performance of grass filters under laboratory and C
C field Conditions".Trans. ASAE, 27(5):1321-1331, to account for C
C triangular upslope deposition and particle and size distribution C
C 6. Wilson et al (1981)"A Hydrology and sedimentology model: Part I. C
C Modeling techniques. U.of Kentucky. Lexington. This is a major C
C rewrite of the prodedures involved. C
C 7. Haan et al (1994)"Design Hydrology and Sedimentology for Small C
C Catchments". Prentice-Hall. Chapter 9C contains updated and clearly C
C presented procedures for sediment trapping and wedge formation C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C SUBROUTINES BY ORDER OF APPAREANCE C
C
C INI, INPUTS,QUAD, FORMA, SHAPEF, ASSM, BCA, FORMB, MODIFY, FACTOR, C
C SOLVE, FLOW, UPDATE, CONVER, KVVWRITE, GASUB, OUTMASS, GRASSED, C
C GRASSIN, OCF, EINSTEIN, STEP3, POINTS C
C
C DEFINITION OF GLOBAL VARIABLES FOR OVERLAND FLOW SOLUTION C
C
C A(I,J)= SYSTEM MATRIX, SQUARE OF DIMENSIONS NxN, ie. [A] C
C B(I)= RIGHT HAND SIDE VECTOR OF DIMENSIONS 1xN , ie {b} C
C DPSI(L) = DERIVATIVE OF BASIS FUNCTIONS C
C DR= DURATION OF THE RAINFALL (s) C
C DT = INCREMENT OF TIME (s) C
C DX= SPACE STEP (m) C
C MAXITER= MAXIMUM NUMBER OF ITERATIONS ALLOWED C
C MFLAG= CONVERGENCE FLAG (0, NO CONVERGENCE; 1, CONVERGENCE) C
C N=ACTUAL NUMBER OF NODES IN THE DOMAIN C
C NDT = NUMBER OF TIME STEPS C
C NELEM= ACTUAL NUMBER OF ELEMENTS IN THE DOMAIN C
C NL= ORDER OF THE INTEGRATION RULE OVER EACH ELEMENT C
C NMAX= MAXIMUM NUMBER OF EQUATIONS AND VARIABLES THAT CAN BE SOLVED C
C NPOL=NUMBER OF NODAL POINTS OVER EACH ELEMENT (POLYNOMIAL DEG +1) C
C OUT= 0, print values at the downstream end of the plane (hydrograph) C
C 1, Print values for all nodes at each time step C
C QK(MAXEQN)= NODAL ALPHA IN MANNING'S UNIFORM FLOW EQUATION C
C R= Lateral inflow (m/s) C
C RN = MANNING'S ROUGHNESS COEFFICIENT C
C SO = SLOPE OF THE ELEMENT C
C SR= DURATION OF THE SIMULATION (s) C
C THETAW= TIME-WEIGHT FACTOR C
C VL= LENGTH OF THE PLANE (m) C
C W(L) = GAUSS QUADRATURE WEIGHTS C
C X(I)= SOLUTION VECTOR, DIMENSION 1xN, AT TIME STEP L+1 C
C XI(L)= GAUSS QUADRATURE POINT C
C XM(I)= SOLUTION VECTOR, DIMENSION 1xN, AT ITERATION M, t STEP L+1 C
C X0(I)= SOLUTION VECTOR, DIMENSION 1xN, AT TIME STEP L C
C
C
C DEFINITION OF GLOBAL VARIABLES FOR INFILTRATION SOLUTION C
C
C AGA = Green-Ampt's "A", saturated hydraulic conductivity, Ks (m/s) C

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C BCROFF(200,2)= Boundary condition at the upstream node (inflow from C
C adjacent field. C
C BGA = Green-Ampt's "B" = Ks*Sav*M (m2/s) C
C CP= Chu's surface condition indicator for ponding at initial time C
C CU= Chu's surface condition indicator for no-ponding at initial time C
C F= Cumulative infiltration (m) C
C FPI= Instantaneous infiltration rate (m/s) C
C L= rainfall period C
C LO = index to show if time step is in the same rainfall period (LO=L) C
C NPOND= shows ponded (=1) non-ponded (=0) surface conditions C
C NEND= Indicates that the end of runoff is reached C
C PS= Cumulative recipitation in m. C
C PSOLD= Cumulative recipitation in m for last rainfall period. C
C PST= Total cumulative recipitation in m. C
C PSI(L) = BASIS FUNCTIONS (QUADRATIC LAGRANGIAN POLYNOMIALS) C
C RAIN(200,2)= Times (s) and rainfall rates (m/s) over the VFS. C
C RO= Cumulative runoff rate at the node (without considering BCRO) C
C SM= Maximum surface storage (m) C
C STO= Cumulative surface storage (m) C
C TP, TPP= Chu's (1978) tp and tp' coefficients C
C TI= time to infiltrate surface ponded water C
C TRAI= Total cumulative rainfall (m) C
C
C DEFINITION OF VARIABLES FOR SEDIMENT SOLUTION C
C
C Ss= spacing of the filter media elments (cm) C
C Sc= filter main slope C
C n= Manning's n= 0.0072 for cilindrical media (s/cm^1/3) C
C q= overland flow (cm2/s) C
C df= depth of flow at D(t) (cm) C
C Vm= depth averaged velocity at D(t)(cm/s) C
C Rs= hydraulic radius of the filter (cm) C
C dp= particle size, diameter (cm) C
C gamma, gammas= water and sediment weight density (g/cm3) C
C gs2=gsd: sediment load entering downstream section (g/s/cm) C
C Rss= hydraulic radius of the filter at B(t) (cm) C
C dfs= depth of flow at B(t) (cm) C
C Vms= depth averaged velocity at B(t) (cm/s) C
C Se= equilibrium slope at B(t) C
C f= fraccion trapped in the depodition wedge C
C ico= flag to select feedback to overland flow solution of new slopes C
C and roughness (0=no, 1=yes) C
C coarse= % of particles from incoming sediment with diameter > 0.0037 C
C cm (coarse fraction that will be routed through wedge). C
C
C NOTE: units in sediment transport calculations are in CGS system C
C (cm,g,s), including Manning's n C
C
c Change Log: See CHANGES file in source code directory c
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
PARAMETER (MAXEQN=1001,MAXBND=40)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)

COMMON/PAR/QK(200),R,THETAW,DX,DT,NDT,NELEM,MAXITER,NPOL,IOUT,NL
COMMON/GA1/PS,PSOLD,PST,F,RO,TP,TPP,TI,FPI,STO,CU,CP,AGA,BGA,SM
COMMON/GA2/LO,NPOND
COMMON/GRASSD/PART(3),SC,SS,VN1,VN2,VN,GSI,H,VLCM,POR,CI,ICO
COMMON/GRASSD2/GSIMASS,GSOMASS,TTE,DEP,QSED(4),RS(3),DF(3),VM(3)
COMMON/GRASSD3/SUSMASS,WEDGEMASS,NFUP
COMMON/OLD/SEOLD,GSIOLD,FOLD,TOLD,XTOLD,YTOLD,CDEP,SE,VBTOLD
COMMON/FLOWPAR/X0,Q0
DIMENSION A(MAXEQN,MAXBND),B(MAXEQN),B0(MAXEQN)
DIMENSION X(MAXEQN),X0(MAXEQN),XM(MAXEQN),Q0(MAXEQN),QM(MAXEQN)
DIMENSION PGPAR(4)
DIMENSION BCROFF(200,2),RAIN(200,2),NODEX(4)
CHARACTER*75 LISFIL(13)

```

C-----Print banner, get I/O filenames and open them -----

```

CALL FINPUT(LISFIL,INARGS,ISCR)

C-----Initialize matrices-----

CALL INI(A,B,X,XM,X0,Q0,QM,SSE,NODEX)

C-----Read inputs for sediment problem-----

CALL GRASSIN(ICOARSE,COARSE,LISFIL,INARGS)

C----Get inputs and parameters for hydrology problem-----

CALL INPUTS(N,NBAND,NRAIN,RAIN,NBCROFF,BCROFF,TE,QMAX,VL,FWIDTH,
& SWIDTH,SLENGTH,PGPAR,NCHK,LISFIL,INARGS,ISCR,IWQ)

C-----Get the Gauss quadrature parameters-----

CALL QUAD

C-----Assemble the system matrix A -----

CALL FORMA(A,NBAND,PGPAR)

C-----Perform LU decomposition over A -----

CALL FACTOR(A,N,NBAND)

C-----Numerical time dependent solution-----

MAXIT=100
TIME=0.D0
RO=0.D0
PS=0.D0
STO= 0.D0
F=0.000001D0
XTOLD=0.D0
YTOLD=0.D0
TOTF=0.d0
NPOND=0
PZERO=1.0d-8
NSTART=0
NEND=0
NWRITE=NDT/100
VLCM=VL*100.D0
QTEMP=0.d0
NFUP=0
MMX=0
! added GSO for grassed-->step3-->SedLoadTRT
! Initializing GSO to 0.0
GSO=0.d0
YT=0.d0
XT=0.d0
! iTRTcount is used if tarse is called.
iTRTcount=1

DO 5 I=1,4
  QSED(I)=0.D0
5  CONTINUE
DO 40 LCOUNT=1,NDT
  TIME=DT*LCOUNT

C----- Select the rainfall intensity and interpolate BC (transform into depth (m)) ---
C----- at the first node of system (incoming hydrograph) for each time step.

R=0.D0
DO 10 I=1,NRAIN-1
  IF(TIME.GT.RAIN(I,1).AND.TIME.LE.RAIN(I+1,1)) L=I
10  CONTINUE
BCRO=0.D0
BCROQ=0.D0

```

```

DO 15 I=1,NBCROFF-1
IF(TIME.GT.BCROFF(I,1).AND.TIME.LE.BCROFF(I+1,1)) THEN
  BCROQ=(TIME-BCROFF(I,1))/(BCROFF(I+1,1)-BCROFF(I,1))*
  & (BCROFF(I+1,2)-BCROFF(I,2))+BCROFF(I,2)
  BCRO=((BCROQ/FWIDTH)/QK(1))**(3.D0/5.D0)
ENDIF
15 CONTINUE

C----- Get effective rainfall and control execution of overland flow----
C----- for an infiltrating surface by calling Green-Ampt model. The ---
C----- assumption is that when a certain node (nchk) is flooded, i.e. --
C----- x(nchk)>0, all the surface will be flooded, and thus the max. ---
C----- infiltration capacity for the rest of the event is selected -----
C-----as given by the Green-Ampt model. NCHK is selected by the user.--

  IF(X(NCHK).GT.PZERO)NPOND=1
  IF(BCRO.EQ.0.D0.AND.X(NCHK).EQ.0.D0.AND.NSTART.EQ.1)NEND=1
C-----consider infiltration for infiltrating plane (mod for thetai>porosity 05/2003)---
  IF(AGA.GT.0.D0)THEN
C-----change to consider infiltration only when rainfall occurs -----
C  IF(AGA.GT.0.D0.AND.R.GT.0.0000E+00)THEN
C-----end of change -----
  CALL GASUB(TIME,DT,L,R,RAIN,NEND,TRAI)
  ELSE
    R=RAIN(L,2)
    TRAI=TRAI+DT*(R+ROLD)*0.5D0
    ROLD=R
  ENDIF
  IF(R.LE.0.D0.AND.BCRO.EQ.0.D0.AND.X(NCHK).EQ.0.D0)NSTART=0
  IF(R.GT.0.D0.OR.BCRO.GT.0.D0)NSTART=1

C-----Form of r.h.s vector for that time step -----

  CALL FORMB(B0,X0,Q0,N,BCRO,PGPAR)

C-----Start Picard iteration-----

  M=0
  MFLAG=0
  IF(NSTART.EQ.0)MFLAG=1
  DO 20 WHILE (M.LT.MAXITER.AND.MFLAG.EQ.0)
    M= M+1

C-----Update {b} = {bm} -----

    CALL UPDATE(N,B0,B)
    CALL MODIFY(QM,B,BCRO,PGPAR)

C-----Feed the vector to the solver-----

    CALL SOLVE(A,B,X,N,NBAND)

C-----Check for convergence-----

    CALL CONVER(N,X,XM,MFLAG)

C-----Update Xm = X m+1 -----

    CALL UPDATE(N,X,XM)

C-----Find flow component at iteration step-----

    CALL FLOW(N,X,QM)

20 CONTINUE

C-----Update h and q for next time level-----

  CALL UPDATE(N,X,X0)
  CALL FLOW(N,X,Q0)

```

C-----Do the following only 100 times, each time using the ----
 C-----average flow of the last NWRITE values in between -----
 C-----a) Call sediment transport subroutine if there is inflow--
 C----- (change units from q(m2/s)-->qsed(cm2/s))-----
 C-----b) Write outputs to files -----

```

    QTEMP=QTEMP+Q0(N)
    DO 25 J=1,3
      ND=NODEX(J)
      QSED(J)=QSED(J)+Q0(ND)
25  CONTINUE
    DO 30 I=1,100
      IF(LCOUNT.EQ.I*NWRITE) THEN
        QTEMP=QTEMP/NWRITE
        DO 27 J=1,3
          QSED(J)=QSED(J)/NWRITE*10000.D0
          IF(QSED(J).LT.0.D0)QSED(J)=DABS(QSED(J))
27  CONTINUE
        QSED(4)=QTEMP*10000.D0
        QIN=QK(1)*BCRO*(5.D0/3.D0)*10000.D0
        QOUT=Q0(N)

        IF(BCRO.NE.0.D0) THEN
          CALL GRASSED(TIME,N,QIN,QOUT,NODEX,
&          ICOARSE,COARSE,FWIDTH,ISCR,GSO)
        ENDIF
        TOLD=TIME
        CALL KWWRITE(N,LCOUNT,M,QTEMP,X,BCROQ,FWIDTH)
        QTEMP=0.D0
        DO 28 J=1,4
          QSED(J)=0.D0
28  CONTINUE
        ENDIF
30  CONTINUE
      IF (IWQ.EQ.1) then
        FPI=-1*(R-RAIN(L,2))
        rainWQ=RAIN(L,2)
        if (Q0(1).GT.0) then
          call WQSUB(TIME,NBAND,N,LISFIL,iTRTcount,Lcount,FPI,RAINWQ)
          MMX=1
        else

          if (MMX.EQ.1)
&          call WQSUB(TIME,NBAND,N,LISFIL,iTRTcount,Lcount,FPI,RAINWQ)
          end if
        END IF

      NNWRITE=NDT/5
      DO 50 Ip=1,5
        IF(LCOUNT.EQ.Ip*NNWRITE) THEN
          iprogress=20*Ip

          print *, "Progress: ",iprogress,'% '

        END IF
50  CONTINUE

40  CONTINUE

```

C-----Write a summary of results at the end of the run --

```

CALL OUTMASS(VL,FWIDTH,SWIDTH,SLENGTH,TRAI,LISFIL,ISCR,IWQ)

CLOSE(1)
CLOSE(2)
CLOSE(3)
CLOSE(7)
CLOSE(8)
CLOSE(9)

```



```

IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON/PAR/QK(200),R,THETAW,DX,DT,NDT,NELEM,MAXITER,NPOL,IOUT,NL
COMMON/WQ1/VKD,CCP,IWQPRO
COMMON/RSE3/Atrt,Atr2,Atr3,BMtrt,BMtrt2,BMtrt3,Btrt,Btrt2,Btrt3
CHARACTER*75 LISFIL(13)
DIMENSION Atrt(MAXEQN,MAXBND),BMtrt(MAXEQN,MAXBND) ,Btrt(MAXEQN)
DIMENSION Atrt2(MAXEQN,MAXBND),BMtrt2(MAXEQN,MAXBND),Btrt2(MAXEQN)
DIMENSION Atrt3(MAXEQN,MAXBND),BMtrt3(MAXEQN,MAXBND),Btrt3(MAXEQN)
DIMENSION Xtrt(MAXEQN) ,X0trt(MAXEQN)
DIMENSION Xvfs(MAXEQN)
DIMENSION STAB2(MAXEQN),STAB3(MAXEQN),STAB4(MAXEQN)
DIMENSION STAB5(MAXEQN), STAB6(MAXEQN)
DIMENSION TSED(MAXEQN),FSED(MAXEQN),CSED(MAXEQN),SEDVFS(MAXEQN)
ISPLIT=2
!!SPLIT Used to update DT/2 in formbm,.f and elem.f during TRT

```

```

C Numerical time dependent solution
DT2=0.d0

```

```

C THE TRANSPORT-REACTION-TRANSPORT MODULE IS HERE:
C 1/2 STEP TRANSPORT - FULL STEP REACTION - 1/2 STEP TRANSPOR FOR
C EACH TIME STEP.

```

```

!C Initialize matrices
CALL INItrt(Atrt,BMtrt,Btrt,Xtrt,X0trt,LCOUNT)
!C Assamble the system matrix A
CALL FORMAtrt(Atrt,N,NBAND,ISPLIT,rainWQ)
!C Apply boundary conditions over A
CALL BCAtrt(Atrt,N,NBAND)
!C perform LU decomposition over A
CALL FACTOR(Atrt,N,NBAND)
!C Assemble the R.H.S. matrix BM
CALL FORMBMtrt(BMtrt,N,NBAND,ISPLIT,rainWQ)

```

```

C STARTING 1/2 TIME STEP OF TRANSPORT

```

```

C Form r.h.s vector
CALL FORMVBtrt(BMtrt,X0trt,N,NBAND,Btrt,LCOUNT,DT2)
C Feed the vector to the solver
CALL SOLVE(Atrt,Btrt,Xtrt,N,NBAND)
CinP=Xtrt(1)
c STARTING REACTION
!C Concentration after 1/2 dt of transport is passed to one dt of Reaction
! CHECK if tarse is used (IWQPRO=3 for tarse). if not, RSE is nor used
! but a simple sink/souce term can be used by FEMADRtrt
if (IWQPRO.eq.3) then
CALL REACTION(Xtrt,N,LCOUNT,iTRTcount,LISFIL,FPI)
!!iTRTcount=iTRTcount+1
end if
Xtrt(1)=CinP

```

```

C Update the value Xold=Xnew / Updating concentration after reaction
CALL UPDATE(N,Xtrt,X0trt)

```

```

C STARTING SECOND 1/2 TIME STEP OF TRANSPORT

```

```

C Form r.h.s vector
CALL FORMVBtrt(BMtrt,X0trt,N,NBAND,Btrt,LCOUNT,DT2)
C Feed the vector to the solver
CALL SOLVE(Atrt,Btrt,Xtrt,N,NBAND)
!C Write the solution for that time step
CALL CORRECT(Xtrt,N)
C Update the value Xold=Xnew
CALL UPDATE(N,Xtrt,X0trt)
call CHKtrt(N,X0trt,ConcINF1,ConcINF2)
call CHKtrt(N,Xtrt,ConcINF1,ConcINF2)
Xtrt(1)=CinP
CALL ADRWRITE(Xtrt,N,LCOUNT,TIME,FPI,rainWQ,ConcINF1,ConcINF2)
ConcINF1=0.d0
ConcINF2=0.d0
END

```

```

SUBROUTINE ADRWRITE(Xtrt,N,LCOUNT,TIME,FPI,RAINWQ,ConcINF1,
& ConcINF2)
PARAMETER (MAXEQN=1001,MAXBND=40)

```



```

DIMENSION Atrt2(MAXEQN,MAXBND),BMtrt2(MAXEQN,MAXBND),Btrt2(MAXEQN)
DIMENSION Atrt3(MAXEQN,MAXBND),BMtrt3(MAXEQN,MAXBND),Btrt3(MAXEQN)
DIMENSION TSED(MAXEQN),FSED(MAXEQN),CSED(MAXEQN),SEDVFS(MAXEQN)
DIMENSION STAB2(MAXEQN),STAB3(MAXEQN),STAB4(MAXEQN)
DIMENSION STAB5(MAXEQN), STAB6(MAXEQN)
CHARACTER (len=120)      :: XMLinput
CHARACTER (len=120)      :: XMLoutput
CHARACTER (len=120)      :: XMLreac_set
CHARACTER (len=120)      :: fname
integer(kind=4)          :: ntot, NDT1,iii
integer*1, Dimension (50) :: XMLinputC, XMLoutputC, XMLreac_setC
integer(kind=4)          :: iTRTcount
! Initialize for the first iteration
  if (iii.EQ.1) then
    Do i = 1, 50
      C1(i) = 0.0
    Enddo
! Reads data from .iwq file
    call ReadIWQ2(LISFIL)

! Transform fortran strings to C null-terminated strings
! to be used by RSE dll
    Call FORT_CSTRING(XMLinput, XMLinputC)
    Call FORT_CSTRING(XMLoutput, XMLoutputC)
    Call FORT_CSTRING(XMLreac_set,XMLreac_setC)

! Time step used by the controlling program
    if (dtRSE>0) then
      dt_vfsm=dtRSE
    else
      dt_vfsm=dt_vfsm
    end if
  end if
! nvar+27+: 1) Total Seds, 2) Fine Seds, 3) Coarse Seds, 4) Seds on VFS, 5)Infiltration, 6) runoff depth
  C1(1)=Xj

  if (nstab.eq.1) C1(nmob+1)=STAB2(jj)
  if (nstab.eq.2) then
    C1(nmob+1)=STAB2(jj)
    C1(nmob+2)=STAB3(jj)
  end if
  if (nstab.eq.3) then
    C1(nmob+1)=STAB2(jj)
    C1(nmob+2)=STAB3(jj)
    C1(nmob+3)=STAB4(jj)
  end if
  if (nstab.eq.4) then
    C1(nmob+1)=STAB2(jj)
    C1(nmob+2)=STAB3(jj)
    C1(nmob+3)=STAB4(jj)
    C1(nmob+4)=STAB5(jj)
  end if
  if (nstab.eq.5) then
    C1(nmob+1)=STAB2(jj)
    C1(nmob+2)=STAB3(jj)
    C1(nmob+3)=STAB4(jj)
    C1(nmob+4)=STAB5(jj)
    C1(nmob+5)=STAB6(jj)
  end if

  C1(nvarX+27+1)=TSED(jj)
  C1(nvarX+27+2)=FSED(jj)
  C1(nvarX+27+3)=CSED(jj)
  C1(nvarX+27+4)=SEDVFS(jj)
  C1(nvarX+27+5)=FPI
  C1(nvarX+27+6)=X0(jj)

!Call RSE (number of iter, vector W/data of parameters, dt, XML files(2), reaction set, Total number of indexes (based on XML
output)

```

```

call MyReactionModTest(LLL,C1,dt_vfsm,XMLinputC,XMLoutputC,
& XMLreac_setC,ntot,iii)
xj=C1(1)
if (nstab.eq.1) STAB2(jj)=C1(nmob+1)
if (nstab.eq.2) then
  STAB2(jj)=C1(nmob+1)
  STAB3(jj)=C1(nmob+2)
end if
if (nstab.eq.3) then
  STAB2(jj)=C1(nmob+1)
  STAB3(jj)=C1(nmob+2)
  STAB4(jj)=C1(nmob+3)
end if
if (nstab.eq.4) then
  STAB2(jj)=C1(nmob+1)
  STAB3(jj)=C1(nmob+2)
  STAB4(jj)=C1(nmob+3)
  STAB5(jj)=C1(nmob+4)
end if
if (nstab.eq.5) then
  STAB2(jj)=C1(nmob+1)
  STAB3(jj)=C1(nmob+2)
  STAB4(jj)=C1(nmob+3)
  STAB5(jj)=C1(nmob+4)
  STAB6(jj)=C1(nmob+5)
end if
iii=iii+1
  END

```

```

SUBROUTINE CHKtrt(N,X0trt,ConcINF1,ConcINF2)
! CHECK THE WATER DEPTH IN THE VFS. IF THERE IS NO WATER
! THEN THE CALCULATED CONCENTRATION IN SURFACE WATER IS MOVED TO THE POREWATER
PARAMETER (MAXEQN=1001,MAXBND=40)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON/FLOWPAR/X0,Q0
DIMENSION X0(MAXEQN),Q0(MAXEQN),X0trt(MAXEQN)
ConcINF1=0.d0
ConcINF2=0.d0
j=0
Do 10 i=1,N
  ConcINF1=ConcINF1+X0trt(i)
10 CONTINUE
ConcINF1=ConcINF1/(N-2)

  DO 20 l=1,N
    if (X0(l).GT.0.D0) X0trt(l)=X0trt(l)
      if (X0(l).LE.0.D0) then
        ConcInf2=ConcInf2+X0trt(i)
        X0trt(l)=0.d0
        j=j+1
      end if
20 CONTINUE
if (j.gt.0) then
  ConcINF2=ConcInf2/j
else
  ConcINF2=0.d0
end if
RETURN
END

```

```

SUBROUTINE CORRECT(Xtrt,N)

```

!C WRITE THE RESULT VECTOR X IN FORMAT TO THE DEFAULT DEVICE

PARAMETER (MAXEQN=1001,MAXBND=40)

IMPLICIT DOUBLE **PRECISION** (A-H,O-Z)

DIMENSION Xtrt(MAXEQN)

NVAL=N

DO 10 L=1,NVAL

if (Xtrt(L).lt.0)**then**

Xtrt(L)=0

end if

10 **continue**

RETURN

END

Function DIS(VX1)

IMPLICIT DOUBLE **PRECISION** (A-H,O-Z)

COMMON/PARADR/CONC1,DISL,DISM,CK1

! Calculates the hydrodynamic dispersion coefficient

DIS = VX1*DISL+DISM

return

end

SUBROUTINE ELEMtrt(EK,ISPLIT1,NUMELEM,rainWQ)

!CC C C

!C SUBROUTINE ELEM EVALUATE THE COMPONENTS

!C

!C e x2 e e e e e e e

!C k=Ow[Dx N(x) 'N(x) '+Vx N(x)N(x)+kl N(x)N(x) +N(x)N(x)/dt]dx

!C ij x1 i j i j j i i j

!C

!C FOR THE ELEMENT STIFFNESS MATRIX k.

!C THE TRANSFORMATION FROM c TO X IS GIVEN BY THE RELATION

!C $X = x1 + 1/2(x2 - x1) (1 + c)$

!C THUS

!C e e

!C dN dN dc

!C i i

!C --- = --- ---

!C dx dc dx

!C

!C AND

!C

!C dx x2 -x1 dx1

!C ---- = ---- = ----

!C dc 2 2

!C

!C N -NUMBER OF NODAL POINTS IN THE ELEMENT

!C THETA W -TIME WEIGHTING FACTOR

!C e

!C EK(I,J) -k , ENTRY IN ELEMENT STIFFNESS MATRIX

!C ij

!C NL -ORDER OF THE INTEGRATION RULE

!C X1(L) -cl, THE LOCATION OF THE L-TH GAUSS ABSCISSA

!C W(L) -wl, THE L-TH GAUSS WEIGHT

!C dx x2 -x1

!C DXI/2 = --- = ----- = No. NODES IN ELEMENT TIMES DX/2

!C dc 2

PARAMETER (MAXEQN=1001,MAXBND=40)

IMPLICIT DOUBLE **PRECISION** (A-H,O-Z)

COMMON/CINTtrt/Xltrt(4,4),Wtrt(4,4)

COMMON/PARADR/CONC1,DISL,DISM,CK1

COMMON/PAR/QK(200),R,THETA W,DX,DT,NDT,NELEM,MAXITER,NPOL,IOUT,NL

```

! COMMON/OLD/SEOLD,GSIOld,FOLD,TOLD,XTOLD,YTOLD,CDEP,SE,VBTOld
! COMMON/RSE2/STAB2,ISPLIT
! COMMON/WQ2/IWQPRO,TIME
COMMON/FLOWPAR/X0,Q0
DIMENSION EK(4,4),PSI(4),DPSI(4)
DIMENSION X0(MAXEQN),Q0(MAXEQN)
!C Find the integral domain
DX1=DX*(NPOL-1)
!C Inizialize element arrays
DO 10 I=1,NPOL
    DO 10 J=1,NPOL
        EK(I,J) = 0.D0
10 CONTINUE
!C Begin integration point loop
!NL is adapted for reading a value up to 4
IF (NL.LE.4) THEN
    NL2=NL
    NODE=(NPOL-1)*NUMELEM-NPOL+1
    NODETEMP=NODE

    DO 20 L=1,NL
        NODE=NODETEMP
        CALL SHAPEtrt (Xltrt(L,NL),NPOL,PSI,DPSI)
        DO 20 I=1,NPOL
            NODE=NODE+1
            IF (Q0(NODE).LE.0) THEN
                VX=0.d0
                CK1p=0.d0
            ELSE
                VX=Q0(NODE)/X0(NODE)
                CK1p=rainWQ/X0(NODE)+CK1
            END IF
            DO 20 J=1,NPOL
                EK(I,J) = EK(I,J)+((DIS(VX)*DPSI(I)*DPSI(J)*2.D0/DX1
&&
+VX*PSI(I)*DPSI(J)+CK1p*PSI(I)*PSI(J)*DX1/2.D0)*THETAW
+PSI(I)*PSI(J)*DX1/2.D0/(DT/ISPLIT1))*Wtrt(L,NL)
20 CONTINUE

        ELSE
            NL2=NL
            NL=NL-1
            NODE=(NPOL-1)*NUMELEM-NPOL+1
            NODETEMP=NODE

            DO 30 L=1,NL
                NODE=NODETEMP
                CALL SHAPEtrt (Xltrt(L,NL),NPOL,PSI,DPSI)
                DO 30 I=1,NPOL
                    NODE=NODE+1
                    IF (Q0(NODE)<=0) THEN
                        VX=0.d0
                        CK1p=0.d0
                    ELSE
                        VX=Q0(NODE)/X0(NODE)
&&
! CK1p substitutes CK1 in EK calculations
                        CK1p=rainWQ/X0(NODE)+CK1
                    END IF
                    DO 30 J=1,NPOL
                        EK(I,J) = EK(I,J)+((DIS(VX)*DPSI(I)*DPSI(J)*2.D0/DX1
&&
+VX*PSI(I)*DPSI(J)+CK1p*PSI(I)*PSI(J)*DX1/2.D0)*THETAW
+PSI(I)*PSI(J)*DX1/2.D0/(DT/ISPLIT1))*Wtrt(L,NL)
30 CONTINUE
                END IF
                IF (NL2.GE.5) NL=NL2
            RETURN
        END

SUBROUTINE FORMAttr(Attr,N,NBAND,ISPLIT,rainWQ)
! from femadrTRT CALL FORMAttr(Attr,N,NBAND,ISPLIT)
!C C C This subroutine assembles the system matrix [A] as a banded matrix C

```



```

        CK1p=0
                                DO 32 J=1,NPOL
                                EF(I,J)=EF(I,J)+0
32      CONTINUE
        else
        VX=Q0(NODE)/X0(NODE)
        CK1p=rainWQ/X0(NODE)+CK1
                                DO 34 J=1,NPOL
                                EF(I,J)=EF(I,J)+(PSI(I)*PSI(J)*DX1/2.D0/(DT/ISPLIT)-
(DIS(VX)*DPSI(I)*DPSI(J)*2.D0/DX1+VX*PSI(I)*DPSI(J)
+CK1p*PSI(I)*PSI(J)*DX1/2.D0)*(1-THETAW))*Wtrt(L,NL)
34      CONTINUE
        end if
30      CONTINUE

!C Plug the element vector into the [BMtrt] matrix
        CALL ASSM(BMtrt,EF,NBAND,NEL)
50      CONTINUE
!IC Plug in first kind of BC (Dirichlet)
        NDIAG = NBAND/2 + 1
        DO 60 I=1,NBAND
        BMtrt(1,I)=0.D0
60      CONTINUE
        BMtrt(1,NDIAG)=1.D0
!C Second kind of BC (Neumann)
!C NOTE: In this case since de value is 0 the
!C eq. for the last node remains the same
        if (NL2.gt.4) then
        NL=NL2
        end if
        RETURN
        END

        SUBROUTINE FORMVBtrt(BMtrt,X0trt,N,NBAND,Btrt,LCOUNT,DT2)
!from femadrTRT8t f call FORMVBtrt(BMtrt,X0trt,N,NBAND,Btrt,LCOUNT)
!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
!C AUTHOR: Casson stallings, NCSU, Forestry Department, Spring 1991
!C
!C This Subroutine constructs the r.h.s. vector {b} at every time
!C step as the result of the banded matrix multiplication:
!C
!C          1
!C          {b} = [BM] .{C}
!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
!C
!C          DEFINITION OF GLOBAL VARIABLES
!C N          = NUMBER OF ACTIVE ROWS
!C NBAND      = BAND WIDT
!C Btrt(N)    = RESULTANT VECTOR
!C IDIAG      = THE ROW EQUIVILANT T TO THE FULL MAT DIAG.
!C ISTEP      = A CONVICIENCE
!C SUM        = HOLDS ROW SUMS
!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC~

        PARAMETER (MAXEQN=1001,MAXBND=40)
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        DIMENSION BMtrt(MAXEQN,MAXBND) ,X0trt(MAXEQN),Btrt(MAXEQN)
        COMMON/FLOWPAR/X0,Q0
        COMMON/PARADR/CONC1,DISL,DISM,CK1
        DIMENSION X0(MAXEQN),Q0(MAXEQN)
        IDIAG = (NBAND+1)/2
        ISTEP = IDIAG-1
!C Multiply the top most rows -----
        DO IR=1,ISTEP
        ISKEW = IR -IDIAG
        SUM = 0.0D0
        DO IC=(IDIAG+1-IR),NBAND

```

```

        SUM = SUM + BMtrt(IR,IC) * X0trt(IC+ISKEW)
    END DO !! IC !!
    Btrt(IR) = SUM
END DO !! IR !!
!c Multiply the middle rows of the banded matrix-----
DO IR=(ISTEP+1), (N-ISTEP)
    ISKEW = IR -IDIAG
    SUM = 0.0D0
    DO IC=1,NBAND
        SUM = SUM + BMtrt(IR,IC) * X0trt(IC+ISKEW)
    END DO !! IC !!
    Btrt(IR) = SUM
END DO !! IR !!
!C Multiply the last rows of the banded matrix -----
DO IR= (N-ISTEP+1), N
    ISKEW = IR -IDIAG
    SUM = 0.0D0
    DO IC=1, (IDIAG+(N-IR))
        SUM = SUM + BMtrt(IR,IC) * X0trt(IC+ISKEW)
    END DO !! IC !!
    Btrt(IR) = SUM
END DO !! IR !!
!C Take care of BCI -----
! BC as a constant for C=1 @ t>0
!   Btrt(1)= 0.5

    if (Q0(1).GT.0) Btrt(1)=CONC1
    if (Q0(1).LE.0) Btrt(1)=0.D0
!BC as a funcion Ca+Cb*e^-alpha*t @ t>0,
!!   DT2=DT2+(DT/2)
!!   Btrt(1)= 80+30*exp(-1*LCOUNT*0.005)

!C Take care of BC2 -----
!C NOTE: In this case since de value is 0 the -----
!C eq. for the last node remains the same
    RETURN
END

```

```

    subroutine          FORT_CSTRING(string, array)
c*****
c fstrings.for -- routines for converting between FORTRAN and C character
c   strings.
c
c Mark Showalter, PDS Rings Node, September 2002
c*****

c
c*****
c$ Component_name:
c   FORT_CSTRING (fstrings.for)
c$ Abstract:
c   Converts a FORTRAN character string to a null-terminated byte array,
c   for passage to a C function.
c$ Keywords:
c   UTILITY, FORTRAN_C
c   FORTRAN, INTERNAL, SUBROUTINE
c$ Declarations:
c   subroutine          FORT_CSTRING(string, array, nbytes)
c   character*(*)      string
c   integer*1 array(*)
c   integer*4  nbytes
c$ Inputs:
c   string              character string to convert.
c   nbytes              dimensioned length of byte array.
c$ Outputs:
c   array(1...) string of bytes with terminal null.

```

```

c$ Returns:
c     none
c$ Detailed_description:
c     This subroutine converts a FORTRAN character string to a null-terminated
c     byte array, for passage to a C function. Blank characters at the end of
c     the character string are not considered significant. The string is
c     truncated if necessary to fit into the array.
c$ External_references:
c     none
c$ Examples:
c     none
c$ Error_handling:
c     none
c$ Limitations:
c     The dimensioned length of the byte array must be at least one greater
c     than the effective length of the character string.
c$ Author_and_institution:
c     Mark R. Showalter
c     PDS Rings Node, NASA/Ames Research Center
c$ Version_and_date:
c     1.0: January 1994
c     1.1: September 2002
c$ Change_history:
c     1.1: Modified for compatibility with Absoft FORTRAN for Macintosh OS X.
c*****

```

```

character*(*)      string
integer*1 array(*)
integer*4 nbytes

integer            last, i

```

```

c Search for the last character actually used.
do 100 last = len(string), 1, -1
  if (string(last:last) .ne. ' ') goto 101
100  continue
101  continue

```

```

c Truncate string if necessary
!     if (last .gt. nbytes-1) last = nbytes-1

```

```

c Copy bytes from character string
do 200 i = 1, last
  array(i) = ichar( string(i:i) )
200  continue

```

```

c Append null terminator
array(last+1) = 0

return
end

```

```

SUBROUTINE GRASED(TIME,N,QIN,QOUT,NODEX,ICOARSE,COARSE,
& FWIDTH,ISCR,GSO)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     This subroutine solves the sediment transport problem on a grass filter C
C     It utilizes the method proposed by: C
C
C 1. Tollner et al. (1976). "Suspended sediment filtration capacity of C
C     simulated vegetation". Trans. ASAE. 19(4):698-682. C
C 2. Tollner et al. (1977). "Sediment deposition patterns in simulated C
C     grass filters". Trans. ASAE. 20(5):940-944. C
C 3. Barfield et. al (1979)"Filtration of sediment by simulated vegetation C
C     I. Trans. ASAE, 22(3):540-548. C
C 4. Hayes et. al (1979)"Filtration of sediment by simulated vegetation II" C

```



```

DO 10 NPLACE=1,3
  CALL OCF(NPLACE)
10 CONTINUE

C-----STEP 2: Solve Einstein's equation to find transport capacity (gs2)--
C----- at the end of B(t) -----
  CALL EINSTEIN(GS2,NTRCAP,COARSE)
  IF(ICOARSE.EQ.0)NTRCAP=1

C-----STEP 3: Calculate shape of sediment wedge, sediment outflow, and ---
C----- trapping efficiency for the filter and finishes up-----

  CALL STEP3(GS2,TIME,NTRCAP,COARSE,QOUT,FWIDTH,ISCR,YT,XT,GSO,FI,FRAC)

C-----STEP 4: Position points (1), (2), (3) at system nodes so that flow --
C----- rates can be read at those points at next time step -----

  CALL POINTS(N,XPOINTS,NODEX,VBT)
c-----Pass values of Sediment Conc to TSED, FSED and CSED-----
  CALL SedLOADTRT(COARSE,YT,XT,GS2,GSO,FWID,NODEX,XPOINTS,N,FI,FRAC)
C-----Write outputs of sediment transport calculations -----
120 WRITE(14,200)TIME,QIN,(QSED(J),RS(J),VM(J),DF(J),J=1,3),QSED(4)

180 FORMAT(f7.0,4F10.3,F10.6,13E10.3)
200 FORMAT(F7.0,14E10.3)
201 FORMAT(A32,F8.4,a4)
RETURN
END

```

```

SUBROUTINE INItrt(Atrt,BMtrt,Btrt,Xtrt,X0trt,iter)
!from femadrTRT CALL INItrt(Atrt,BMtrt,Btrt,Xtrt,X0trt,iter)

```

```

!C C C SET ALL MATRICES=O TO START PROGRAM C C C

```

```

PARAMETER (MAXEQN=1001,MAXBND=40)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DIMENSION Atrt(MAXEQN,MAXBND),BMtrt(MAXEQN,MAXBND),Btrt(MAXEQN)
DIMENSION Xtrt(MAXEQN),X0trt(MAXEQN)
DIMENSION STAB2(MAXEQN),STAB3(MAXEQN),STAB4(MAXEQN),
& STAB5(MAXEQN), STAB6(MAXEQN)
DIMENSION TSED(MAXEQN),FSED(MAXEQN),CSED(MAXEQN),SEDVFS(MAXEQN)
temp_dt=0 !For RSE if needed
DO 10 I=1,MAXEQN
  if (iter.LE.1) then
    Btrt(I)= 0.D0
    Xtrt(I)= 0.D0
    X0trt(I)=0.D0
    STAB2(I)=0.D0
    STAB3(I)=0.D0
    STAB4(I)=0.D0
    STAB5(I)=0.D0
    STAB6(I)=0.D0
    TSED(I)=0.D0
    FSED(I)=0.D0
    CSED(I)=0.D0
    SEDVFS(I)=0.D0
  end if
  DO 10 J=1,MAXBND
    Atrt(I,J)= 0.D0
    BMtrt(I,J)=0.D0
10 CONTINUE
RETURN
END

```

```

SUBROUTINE INPUTS(N,NBAND,NRAIN,RAIN,NBCROFF,BCROFF,TE,QMAX,VL
& ,FWIDTH,SWIDTH,SLENGTH,PGPAR,NCHK,LISFIL,INARGS,ISCR,IWQ)

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C          C
C Read data from input file *.iwq in free format calculate the C
C following parameters: C
C          C
C 1- N, NBAND,NELEM C
C 2- Maximum flow rate and depth at steady-state condition (QMAX,HMAX) C
C 3- Celerity of the wave (C) C
C 4- Courant time step (DTC) C
C 5- Froude number (FR) C
C 6- Kinematic flow number (FK) C
C 7- Henderson's time to equilibrium (TE) C
C          C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

```

```

PARAMETER (MAXEQN=1001,MAXBND=40)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
CHARACTER*30 PLABEL
CHARACTER*75 LISFIL(13)
CHARACTER*1 CWQ

```

```

COMMON/GA1/PS,PSOLD,PST,F,RO,TP,TPP,TI,FPI,STO,CU,CP,AGA,BGA,SM
COMMON/PAR/QK(200),R,THETA,W,DX,DT,NDT,NELEM,MAXITER,NPOL,IOUT,NL
COMMON/GRASSD/PART(3),SC,SS,VN1,VN2,VN,GS1,H,VLCM,POR,CI,ICO

```

```

COMMON/WQ1/VKD,CCP,IWQPRO
! COMMON/WQ2/IWQPRO,TIME
! COMMON/OLD/SEOLD,GS1OLD,FOLD,TOLD,XTOLD,YTOLD,CDEP,SE,VBTOLD
COMMON/PARADR/CONC1,DISL,DISM,CK1

```

```

DIMENSION BCROFF(200,2),RAIN(200,2)
DIMENSION NODEP(MAXEQN),RNA(MAXEQN),SOA(MAXEQN),SX(MAXEQN)
DIMENSION PGPARR(4)

```

C-----Read in main parameters of the program-----

```

IF(INARGS.EQ.1) THEN
WRITE(*,(' ... Reading inputs from: ',A45))LISFIL(1)
ENDIF
READ(1,*(A30))PLABEL
READ(1,*)FWIDTH
READ(1,*)VL,N,THETA,W,CR,MAXITER,NPOL,IOUT,KPG
IOUT=0

```

C--[EVR-1998]-Check if N is compatible with type of shape function ----

```

L=N-1
M=NPOL-1
IF (MOD (L,M).NE.0) N = N+M-MOD(L,M)
SEPN = VL/(N-1)

```

c----- Read surface properties of the filter -----

```

READ(1,*)NPROP
DO 5 IPROP=1,NPROP
READ(1,*)SX(IPROP),RNA(IPROP),SOA(IPROP)
5 CONTINUE

```

c--[06/2008]-Read WQ flag (0= no; 1= yes) -----

```

READ(1,*,END=8)CWQ
IWQ=INDEX(CWQ,'1')
IF(IWQ.NE.1) IWQ=0

```

C--[EVR-1998]-Assign nodes to the X-values where filter changes ----

```

8 XSEG=0.d0
J = 1
DO 80 I= 1, N
DO WHILE (XSEG.GT.SX(J).AND.I.NE.N)
J= J+1

```

```

                NODEP(J-1)=I
            END DO
            XSEG = XSEG + SEPN
80    CONTINUE
        NODEP(NPROP)=N

```

C ----Calculate alpha for Manning's equation-----

```

SMALLQK=1000.D0
BIGQK=0.D0
SOAVG=0.D0
RNAVG=0.D0
DO 15 I=1,N
    DO 10 IPROP=1,NPROP
        IF(I.LE.NODEP(IPROP))THEN
            RN=RNA(IPROP)
            SO=SOA(IPROP)
            GOTO 12
        ENDIF
    CONTINUE
10    SOAVG=SOAVG+SO
12    RNAVG=RNAVG+RN
    QK(I) = SO*0.5D0/RN
    BIGQK=DMAX1(BIGQK,QK(I))
    SMALLQK=DMIN1(SMALLQK,QK(I))
    IF (QK(I).eq.BIGQK)then
        nbig=i
    ELSEIF (QK(I).eq.SMALLQK)then
        nsmall=1
    ENDIF
15    CONTINUE

```

c-----Filter main slope and roughness for sediment calculations -----

```

SC=SOAVG/N
VN1=RNAVG/N

```

C-----Read rainfall distribution -----

```

IF(INARGS.EQ.1) THEN
    WRITE(*,(' ... Reading inputs from: ",A45')LISFIL(2)
ENDIF
READ(2,*)NRAIN, RPEAK
TOTRAIN=0.d0
DO 20 I=1,NRAIN
    READ(2,*)(RAIN(I,J),J=1,2)
c** fix jep, 10/16/1999
    IF (I.GT.1) TOTRAIN=TOTRAIN+
1    RAIN(I-1,2)*(RAIN(I,1)-RAIN(I-1,1))
20    CONTINUE

DR1=RAIN(NRAIN,1)

```

C-----Calculate Green-Ampt parameters-----

```

IF(INARGS.EQ.1) THEN
WRITE(*,(' ... Reading inputs from: ",A45')LISFIL(4)
ENDIF
READ(7,*)VKS, Sav, OS, OI, SM,SCHK
DM=OS-OI
IF(DM.LE.0.d0)DM=0.0000001d0
IF(VKS.LT.0.d0) VKS=0.d0
SavM=Sav*DM
AGA= VKS
BGA= VKS*SAVM

```

C-----get downslope node for flood checking-----

```

NCHK=IDNINT(SCHK*N)

```

```
IF(NCHK.LT.1)NCHK=1
```

```
C-----Read runoff inflow at upper side of strip (BC) in (m3/s) ---
```

```
IF(INARGS.EQ.1) THEN
WRITE(*,(' ... Reading inputs from: ',A45))LISFIL(3)
ENDIF
READ(3,*)SWIDTH,SLENGTH
READ(3,*)NBCROFF,BCROPEAK
DO 30 I=1,NBCROFF
30 READ(3,*)(BCROFF(I,J),J=1,2)
CONTINUE
DR2=BCROFF(NBCROFF,1)
DR=DMAX1(DR1,DR2)
```

```
C-----Find the bandwidth for the matrix, #element, #nodes---
```

```
NBAND=2*NPOL-1
DX=VL/(N-1)
NELEM=(N-1)/(NPOL-1)
```

```
C-----Calculate convergence and wave form parameters-----
```

```
C***** English Units
c G=32.185D0
c CMN=1.486D0
C***** Metric Units, PEAK & RPEAK (m/s), BCROPEAK (m3/s), QMAX(m2/s)----
G=9.81D0
CMN=1.D0
VMN=5.D0/3.D0
PEAK=RPEAK+BCROPEAK/(VL*FWIDTH)
QMAX= VL*PEAK
HMAX= (QMAX/BIGQK)**(1.D0/VMN)
VMAX=QMAX/HMAX
FR=VMAX/(G*HMAX)**0.5D0
FK=(VL*SO*G)/VMAX**2.D0
C= VMN*BIGQK*HMAX**(VMN-1.D0)
DTC= DX/C
DT=DTC*CR
TE= HMAX/PEAK
NDT=IDINT(DR/DT)
CRR=(VMN*qmax*dt/dx)/((QMAX/SMALLQK)**(1.D0/VMN))
```

```
C-----Calculate the PG Parameters (in this case for n=50)-----
```

```
IF(KPG.EQ.1)THEN
& PGPAR(1)=0.0215873D0 - 0.345217D0*CR + 1.33259D0*CR**2.D0 -
& 1.62016D0*CR**3.D0 + 0.670333D0*CR**4.D0
& PGPAR(2)= 0.0592655D0 - 0.107237D0*CR + 0.235216D0*CR**2.D0 -
& 0.426017D0*CR**3.D0 + 0.222228D0*CR**4.D0
& PGPAR(3)=0.0280422D0 + 0.175632D0*CR - 0.592941D0*CR**2.D0 -
& 0.149698D0*CR**3.D0 - 0.0704731D0*CR**4.D0
& PGPAR(4)= -0.0456247D0 +0.00112745D0*CR +0.420433D0*CR**2.D0 -
& 0.0935913D0*CR**3.D0 - 0.0764558D0*CR**4.D0
ENDIF
```

```
C-----Set the order of the integration rule-----
```

```
IF(KPG.EQ.0.OR.(PGPAR(4).EQ.0.D0.AND.PGPAR(3).EQ.0.D0))THEN
NL=NPOL+1
ELSE
NL=5
ENDIF
```

```
C-----[06/2008]-Read water quality parameters, ensure backwards compatibility ---
```

```
IF(IWQ.EQ.1) THEN
IF (INARGS.EQ.1) THEN
WRITE(*,(' ... Reading inputs from: ',A45))LISFIL(12)
```

```

ENDIF
OPEN(17,FILE=LISFIL(12),ERR=1500,STATUS='OLD')
OPEN(18,FILE=LISFIL(13),STATUS='UNKNOWN')
WRITE(18,220)LISFIL(13)
write(15,225) 12,'iwq',lisfil(12)
write(15,225) 13,'owq',lisfil(13)
READ(17,*)IWQPRO
IF(IWQPRO.EQ.1) THEN
  READ(17,*)IKD
  BACKSPACE(17)
  IF(IKD.EQ.1) THEN
    READ(17,*)IKD,VKOC,OCP
    READ(17,*)CCP
    VKD=VKOC*OCP*.01D0
  ELSE
    READ(17,*)IKD,VKD
    READ(17,*)CCP
  ENDIF
ELSE
ENDIF
ELSE
C
c ----- placeholder for other wq problems, i.e. TaRSE, 07/28/08 rmc
      IF(IWQPRO.EQ.2.OR.IWQPRO.EQ.3) THEN !this initiates reactive term
!      OPEN(31,FILE='femadr.out',STATUS='UNKNOWN')
C Get parameters for running FEMADR or RSE
      CALL INPUTStrt(N,NBAND,IWQPRO)
C Get the Gauss quadrature parameters
      CALL QUADtrt
!      CALL trtON(N,NBAND,IWQPRO) !Reads variables (.iwq file)
      close(17) !iwq file will be opened again if RSE is used
ENDIF

      ENDIF
      ELSE

      write(15,*)
      write(15,*)
ENDIF

C-----Output all the parameters-----
WRITE(11,*)'Storm parameters'
WRITE(11,*)'-----'
WRITE(11,140)PLABEL
IF(INARGS.EQ.1) THEN
  WRITE(*,130)PLABEL
ENDIF
WRITE(11,180)
WRITE(11,150)
WRITE(11,160)
WRITE(11,180)
DO 35 I=1,NRAIN-1
  WRITE(11,170)I,RAIN(I,1),RAIN(I+1,1),RAIN(I,2)
35 CONTINUE
WRITE(11,180)
WRITE(11,350)'Total rainfall (mm)=' ,TOTRAIN*1000.d0
WRITE(11,400)'Peak rainfall intensity(m/s)=' ,RPEAK
WRITE(11,400)'Peak inflow rate BC (m3/s)=' ,BCROPEAK
WRITE(11,*) (The inflow hydrograph can be found in the',
' OUTPUTS')
WRITE(11,*)
WRITE(11,*)'Filter parameters'
WRITE(11,*)'-----'
WRITE(11,200)'Length of the strip (m)=' ,VL
WRITE(11,200)'Width of the strip (m)=' ,FWIDTH
WRITE(11,200)'Surface characteristics='
WRITE(11,525)
WRITE(11,575)
WRITE(11,525)
DO 40 IPROP=1,NPROP
  IF(IPROP.EQ.1) THEN

```

```

                EX1=0.d0
            ELSE
                EX1=(NODEP(IPROP)-1)*DX
            ENDIF
            EX2=(NODEP(IPROP)-1)*DX
            WRITE(11,550)EX1,EX2,RNA(IPROP),SOA(IPROP)
40      CONTINUE
        WRITE(11,525)
        WRITE(11,*)
C-----Output nodal information if desired (ielout=1)-----
        IF(IELOUT.EQ.1)THEN
            WRITE(11,*)' Elemental information follows (IELOUT=1):'
            WRITE(11,185)
            WRITE(11,186)
            WRITE(11,185)
            DO 45 NEL=1,NELEM
                K=(NPOL-1)*NEL-NPOL+1
                DO 45 I=1,NPOL
                    K=K+1
                    WRITE(11,600)NEL,K,I,QK(K),(k-1)*dx
45          CONTINUE
                WRITE(11,185)
                WRITE(11,*)
            ENDIF

            WRITE(11,*)'Soil parameters'
            WRITE(11,*)'-----'
            WRITE(11,400)'Saturated hydraulic cond.(Ks)=' ,VKS
            WRITE(11,200)'Avg. suction at wet front(Sav)=' ,Sav
            WRITE(11,200)'Sat. soil-water content(Os)=' ,Os
            WRITE(11,200)'Initial soil-water content(Oi)=' ,Oi
            WRITE(11,200)'Initial soil-water deficit (M)=' ,DM
            WRITE(11,400)'Green-Ampt parameters (A,B)=' ,AGA,BGA
            WRITE(11,*)'Node number for flood checking= ' ,NCHK
            WRITE(11,*)
            WRITE(11,*)'Simulation parameters'
            WRITE(11,*)'-----'
            WRITE(11,400)'Length of simulation (s)=' ,DR
            WRITE(11,*)' Order of the basis functions= ' ,NPOL-1
C          WRITE(11,*)' Output option (0=q@t;1= h@x)=' ,IOUT
            WRITE(11,700)'Petrov-Galerkin parameters=' ,(PGPAR(I),I= 1,4)
            WRITE(11,200)'Time weighting parameter=' ,THETAW
            WRITE(11,200)'Space step, dx(m)=' ,DX
            WRITE(11,200)'Time step, dt (s)=' ,DT
            WRITE(11,*)'Number of nodes in system =',N
            WRITE(11,*)'Number of elements in system =' ,NELEM
            WRITE(11,*)'Number of time steps =',NDT
            WRITE(11,*)'Maximum number of iterations =' ,MAXITER
            WRITE(11,200)'Maximum flow rate and depth=' ,QMAX,HMAX
            WRITE(11,200)'Celerity of the wave=' ,C
            WRITE(11,200)'Courant time step=' ,DTC
            WRITE(11,200)'Froude number=' ,FR
            WRITE(11,200)'Kinematic wave number=' ,FK
            WRITE(11,200)'Courant number=' ,CR
            IF(IC0.EQ.0)THEN
                WRITE(11,201)'Surface changes feedback=' , NO'
            ELSE
                WRITE(11,201)'Surface changes feedback=' , YES'
            ENDIF
            WRITE(11,*)
C-----Output all input values for sediment transport-----
            WRITE(13,*)'Filter parameters for sediment transport'
            WRITE(13,*)'-----'
            WRITE(13,800)'          Filter main slope (Sc)=' ,SC
            WRITE(13,800)'          Filter media spacing (Ss)=' ,SS,'cm'
            WRITE(13,800)' Modified Manning coefficient (n)=' ,VN,'s.cm^- .33'
            WRITE(13,800)' Manning coeff. for bare soil (n2)=' ,VN2,'s.m^- .33'
            WRITE(13,800)'          Filter media height (H)=' ,H,'cm'
            WRITE(13,*)
            WRITE(13,1050)

```

```

IF(ISCR.EQ.0) THEN
    WRITE(13,1060)
ELSE
    WRITE(13,1061)
ENDIF
WRITE(13,1070)

```

C-----Issue a warning if any of the criteria is not met-----

```

IF(FK.LT.10.D0) THEN
    WRITE(*,*)'WARNING: Kinematic number smaller than 10'
ELSE IF (FR.GT.1.5D0) THEN
    WRITE(*,*)'WARNING: Froude number greater than 2'
ELSE IF (CR.GT.1.D0) THEN
    WRITE(*,*)'WARNING: Courant number greater than 1'
ENDIF
WRITE(11,*)

```

C-----Print header for output values-----

```

IF(IOUT.EQ.0.D0) THEN
    WRITE(11,190)
    WRITE(11,192)
    WRITE(11,198)
    WRITE(11,500)0.d0,0.d0,BCROFF(1,2),0.d0,0.d0,0.d0,0
ELSE
    WRITE(11,194)
    WRITE(11,196)
WRITE(11,198)
ENDIF

```

c-----Output all input values for Water Quality (if IWQ=1)-----

```

IF(IWQ.EQ.1) THEN
    IF(IWQPRO.EQ.1) THEN
        WRITE(18,*)
        WRITE(18,*)'Parameters for Water Quality'
        WRITE(18,*)'-----'
        WRITE(18,201)'      Type of problem=',
& ' Pesticide trapping (BAYER)'
        WRITE(18,800)'Partition coefficient (Kd)=',VKD,'L/Kg'
        WRITE(18,800)' % Clay in sediment (%CL)=',CCP,'%
    ELSE
IF (IWQPRO.EQ.2) then
WRITE(18,201)'Type of problem= FEM fully coupled'
WRITE(18,201)'
WRITE(18,201)'-----Pollutant Parameters-----'
WRITE(18,800)'Concentration in runoff from Source Area: ',
& CONC1,' g/m^3'
WRITE(18,800)'Longitudinal Dispersion: ', DISL,' m'
WRITE(18,800)'Molecular diffusion: ',DISM,' m^2/s'
WRITE(18,800)'Decay coefficient:',CK1,' s^-1'
WRITE(18,201)'
WRITE(18,*)'NODE, TIME (s), Input Load(g/s),
& Output Load (g/s)'
end if
IF (IWQPRO.EQ.3) then
WRITE(18,201)'Type of problem= RSE'
WRITE(18,201)'
WRITE(18,201)'-----Pollutant Parameters-----'
WRITE(18,800)'Concentration in runoff from Source Area: ',
& CONC1,' g/m^3'
WRITE(18,800)'Longitudinal Dispersion: ', DISL,' m'
WRITE(18,800)'Molecular diffusion: ',DISM,' m^2/s'
! WRITE(18,800)'Decay coefficient:',CK1,' s^-1'
WRITE(18,201)'
WRITE(18,*)'NODE, TIME (s), Input Load (g/s),
& Output Load (g/s)'
end if
ENDIF

```

```

! This was deleted to keep IWQ as 1 or 0
! IWQ=IWQPRO
ENDIF

130 FORMAT(1x,'Storm on: ',a30,14x,'...RUNNING...')
140 FORMAT(20x,'Storm data: ',A30)
150 FORMAT(20x,'|Period|',4x,'Time interval',4x,'| Rainfall |')
160 FORMAT(20x,'|',6x,'|',9x,'(s)',9x,'|',3x,'(m/s)',3x,'|')
170 FORMAT(20x,'|',15,'|',F8.1,' to',F8.1,'|',E10.4,' |')
180 FORMAT(20x,'+',6(' '),'+',21(' '),'+',11(' '),'+')
185 FORMAT(20x,3('+',5(' '),'+',9(' '),'+',9(' '),'+')
186 FORMAT(20x,'| Elem| node|local| alpha | x(m) |')
190 FORMAT(3x,'TIME',5x,'OUTFLOW',4x,'CUM.FLOW',5x,'ie =r-f',
& 5x,'INFLOW',4x,'CUM.INFLOW',2x,'ITER')
192 FORMAT(3x,'(s)',6x,'(m3/s)',7x,'(m3)',8x,'(m/s)',6x,'(m3/s)',
& 7x,'(m3)')
194 FORMAT('ITER',6x,'TIME',7x,'INFLOW',6x,'ie =r-f',
& 5x,'DEPTH (X=L/2)')
196 FORMAT(12x,'(s)',10x,'(m)',9x,'(m/s)',9x,'(m)')
198 FORMAT(75(' '))
200 FORMAT(A31,2F12.6)
201 FORMAT(A35,A28)
205 FORMAT(A50)
220 FORMAT('File: ',A40,8x,'VFSMOD v5.0.0 3/2010')
225 format(3x,'File #=',i3,' code:',a3,'=',a)
350 FORMAT(A31,2F12.2)
400 FORMAT(A31,2E12.4)
500 FORMAT(E9.4,5E12.4,I6)
525 FORMAT(20x,'+',21(' '),'+',9(' '),'+',9(' '),'+')
550 FORMAT(20x,'|',F8.4,' to',F8.4,'|',2(F8.4,'|'),E10.4,' |')
575 FORMAT(20x,'|',4x,'x(m) interval',4x,'|',4x,'n',4x,'|',
& 4x,'So',3x,'|')
600 FORMAT(20x,'|',3(I5,'|'),2(F9.4,'|'))
700 FORMAT(A31,4F9.5)
800 FORMAT(A35,F12.6,A11)
1050 FORMAT(' Time Y(t) X1(t) X2(t) L(t)',
& Se gsi gsl gs2 gso Cum.gsi ',
& 'Wedge_mass Lower_mass Cum.gso f frac DEP',
& ' CDEP Tt')
1060 FORMAT(' (s) (cm) (cm) (cm) (cm)',
& '(g/cm.s) (g/cm.s) (g/cm.s) (g/cm.s) (g/cm)',
& '(g/cm) (g/cm) (g/cm) (cm)')
1061 FORMAT(' (s) (cm) (cm) (cm) (cm)',
& '(g/s) (g/s) (g/s) (g/s) (g)',
& '(g) (g) (g) (cm)')
1070 FORMAT('-----',
& '-----',
& '-----',
& '-----')

RETURN

1500 WRITE(*,1600)'ERROR: Input file missing (check project)'
1600 FORMAT(/,A50,/)
STOP
END

SUBROUTINE INPUTStrt(N,NBAND,IWQPRO)
IC C C READ DATA FROM FILE IN.DAT IN FREE FORMAT AND CALCULATE N,NBAND C C C
PARAMETER (MAXEQN=1001,MAXBND=40)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
CHARACTER (len=120) :: XMLinput1,XMLinput
CHARACTER (len=120) :: XMLoutput
CHARACTER (len=120) :: XMLreac_set
CHARACTER (len=120) :: PollutantName

```

```
COMMON/PAR/QK(200),R,THETAW,DX,DT,NDT,NELEM,MAXITER,NPOL,IOUT,NL
COMMON/PARADR/CONC1,DISL,DISM,CK1
```

```
IF (IWQPRO.EQ.2) READ(17,*) CONC1,DISL,DISM,CK1
IF (IWQPRO.EQ.3) then
  read(17,*) XMLinput, XMLoutput, XMLreac_set
  read(17,*) nmob,PollutantName,CONC1,DISL,DISM,CK1
ELSE
ENDIF
NBAND=2*NPOL-1
NELEM=N/(NPOL-1)
NORDER=2*(NPOL-1)+1
if (NL.GT.4) then
NL2=NL
NL=NL-1
end if
IF(NORDER.GT.2*NL-1) THEN
  PRINT*, 'ERROR IN INTEGRATION RULE (FCT.ORDER<=2NL-1) '
  STOP
ENDIF
IF (NL.GT.4)THEN
  PRINT*, 'NL OUT OF RANGE, NL<=4'
  STOP
ENDIF
if (NL2.GT.4) then
NL=NL2
end if
RETURN
END
```

```
SUBROUTINE MyReactionModTest(b,C,dt,XMLinputC2,XMLoutputC2,XMLreac_setC2,numvar,init)
!C This subroutine calls and runs RSE, returning to the hydrodynamic controlling program C
!C the values of the next concentration(s) vector C
!C A forth order RK method is set by default C
use IFPORT
implicit none
Integer(kind=4) :: i, numvar, nstep, b, bt
Real(kind=8), Dimension(50) :: C,C1
Integer(kind=4) :: nvals
Real(kind=8), Dimension(50) :: vars
Integer(kind=4) :: order,init ! Either 2 or 4
Real(kind=8) :: dt
CHARACTER (len=120) :: in_fname
CHARACTER (len=120) :: out_fname
CHARACTER (len=120) :: reac_set
integer*1, Dimension (50) :: XMLinputC2, XMLoutputC2, XMLreac_setC2

!RK order. Pre-set to 4
order = 4
Call runRSE(numvar,C,b,order,dt,XMLinputC2,XMLoutputC2,XMLreac_setC2,init)
C1=C !returns values for next iteration
end
```

```
SUBROUTINE OUTMASS(VL,FWIDTH,SWIDTH,SLENGTH,TRAI,LISFIL,ISCR,
& IWQ)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C C
C This subroutine processes the output hydrograph and find components C
C of the water balance and hydrograph. The results go in "filename.osm" C
C C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
```

```

COMMON/GA1/PS,PSOLD,PST,F,RO,TP,TPP,TI,FPI,STO,CU,CP,AGA,BGA,SM
COMMON/GRASSD/PART(3),SC,SS,VN1,VN2,VN,GS1,H,VLCM,POR,C1,ICO
COMMON/GRASSD2/GSIMASS,GSOMASS,TTE,DEP,QSED(4),RS(3),DF(3),VM(3)
COMMON/GRASSD3/SUSMASS,WEDGEMASS,NFUP
COMMON/OLD/SEOLD,GS1OLD,FOLD,TOLD,XTOLD,YTOLD,CDEP,SE,VBTOLD
COMMON/WQ1/VKD,CCP,IWQPRO
CHARACTER*74 DUMMY
CHARACTER*75 LISFIL(13)

```

C----- Summarize results from filename.ohy file -----

```

CLOSE(11)
CLOSE(13)
OPEN(11,FILE=LISFIL(6),STATUS='OLD')
OPEN(13,FILE=LISFIL(8),STATUS='OLD')
WRITE(10,*)'INPUTS'
WRITE(10,*)'-----'
SUM0=0.D0
SUM1=0.D0
SUM2=0.D0
TIME0=0.D0
READ(11,*)
READ(11,*)
5 READ(11,'(A)')DUMMY
  IDX=INDEX(DUMMY,'ITER')
  IF(IDX.NE.0) GOTO 6
  WRITE(10,*)DUMMY
  GOTO 5
6 READ(11,'(A)')DUMMY
  READ(11,'(A)')DUMMY
  BIG1=0.D0
  NZERO=1
  INI=0
  RAIN_E0=0.D0
  OUTF0=0.D0
  UPIN0=0.D0
  DO 10 I=1,101
    READ(11,*,END=30)TIME1,OUTF1,CUMFLOW,RAIN_E1,UPIN1,CUMIF,NITER
    TIMEINCR=TIME1-TIME0
    AREA0=TIMEINCR*(UPIN1+UPIN0)/2.D0
    SUM0=SUM0 + AREA0
    AREA1=TIMEINCR*(OUTF1+OUTF0)/2.D0
    SUM1=SUM1 + AREA1
    AREA2=TIMEINCR*(RAIN_E1+RAIN_E0)/2.D0
    SUM2=SUM2 + AREA2
    UPIN0=UPIN1
    OUTF0=OUTF1
    RAIN_E0=RAIN_E1
    TIME0=TIME1
    C1= OUTF1
    BIG1=DMAX1(BIG1,C1)
    IF(C1.EQ.BIG1)THEN
      TBIG=TIME1
      QBIG=C1
    ENDIF
    IF(NZERO.EQ.1.AND.C1.GT.0.D0.AND.INI.EQ.0) THEN
      TINI=TIME1
      NZERO=0
      INI=1
    ELSEIF(NZERO.EQ.0.AND.C1.EQ.0.D0) THEN
      NZERO=1
      TEND=TIME1
    ENDIF
    IF(C1.GT.0.D0)TEND=TIME1
10 CONTINUE
  READ(13,*)
  READ(13,*)
12 READ(13,'(A)')DUMMY
  IDX=INDEX(DUMMY,'gs1')
  IF(IDX.NE.0) GOTO 16
  WRITE(10,*)DUMMY

```

```

GOTO 12
16 CONTINUE
WRITE(10,*)'OUTPUTS'
WRITE(10,*)'-----'
30 WRITE(10,*)'Water balance'
WRITE(10,*)'-----'

```

C-----Calculate total rainfall for event in m3 -----

```

TOTRAIN=TRAI*VL*FWIDTH
WRITE(10,600)TOTRAIN
Vout=SUM1
Vie=SUM2*VL*FWIDTH
Vin=SUM0
WRITE(10,300)Vin
WRITE(10,150)Vout

```

C-----Water and sediment balance for the event-----

```

WAT_IN=Vin+TOTRAIN
VF=WAT_IN - Vout
if(AGA.LE.0.D0) VF=0.d0
WAT_OUT= Vout+VF
WAT_BAL=WAT_IN-WAT_OUT
WAT_ERR=WAT_BAL/WAT_IN*100
WRITE(10,400)VF
WRITE(10,*)' '
WRITE(10,*)'Hydrology'
WRITE(10,*)'-----'
WRITE(10,700)TINI
WRITE(10,800)TBIG,QBIG
WRITE(10,900)TEND
WRITE(10,*)' '
WRITE(10,*)'Sediment'
WRITE(10,*)'-----'
TTE=0.D0
IF(GSIMASS.GT.0.D0) TTE=(GSIMASS-GSOMASS)/GSIMASS
FWID=FWIDTH*100.D0
WRITE(10,1100)GSIMASS,GSIMASS*FWID
WRITE(10,1200)GSOMASS,GSOMASS*FWID
WRITE(10,1010)TTE*100

```

c-----Sediment wedge final shape -----

```

WRITE(10,*)' -----'
WRITE(10,1250)
VLT=VLCM-XTOLD
X1=YTOLD/SC
WRITE(10,1300)YTOLD
WRITE(10,1400)XTOLD
WRITE(10,1500)VLT
WRITE(10,1600)X1
WRITE(10,1700)DEP

```

c-----Mass balance -----

```

GAMMASB=(1.D0-POR)*PART(3)
IF(NFUP.EQ.0.AND.YTOLD.LT.H) THEN
c-----Triangular wedge
    BMASS=(DEP*VLT+(XTOLD+X1)*YTOLD*0.5D0)*GAMMASB
    ELSEIF(NFUP.EQ.0.AND.YTOLD.EQ.H) THEN
c-----Trapezoidal wedge
    X3=YTOLD/Se
    X2=XTOLD-X3
    TRBOT=X1+X2+X3
    TRTOP=X2
    BMASS=.5D0*(TRTOP+TRBOT)*YTOLD*gammasb
c-----if strip is filled calculate as rectangle (H*VLCM)
    ELSE
        BMASS=(H*VLCM+(H/SC)*H*0.5D0)*GAMMASB
    ENDF

```

```

WRITE(10,1800)(BMASS-(GSIMASS-GSOMASS))/(GSIMASS-GSOMASS)*100.D0
WRITE(10,1825)WAT_ERR
IF(NFUP.EQ.1) THEN
    WRITE(10,1850)
ELSEIF(YTOLD.EQ.H) THEN
    WRITE(10,1875)
ENDIF

```

c-(02/1999)--Filter performance summary output file -----

```

WRITE(15,*)'
WRITE(15,*)      Summary of Buffer Performance Indicators:'
WRITE(15,*)'
WRITE(15,1900)SWIDTH*SLENGTH
WRITE(15,2000)SLENGTH
WRITE(15,2100)SWIDTH
WRITE(15,2200)VL
WRITE(15,2225)FWIDTH
WRITE(15,2250)VN1
WRITE(15,*)'
WRITE(15,2300)VL/SLENGTH*100.d0
WRITE(15,2400)TOTRAIN/(FWIDTH*VL)*1000.d0
WRITE(15,2450)TOTRAIN
WRITE(15,2500)Vin/(SWIDTH*SLENGTH)*1000.d0
WRITE(15,2550)Vin
WRITE(15,2600)Vout/(SWIDTH*SLENGTH+FWIDTH*VL)*1000.d0
WRITE(15,2650)Vout
WRITE(15,2675)VF
c--- rmc 04/20/03 --Fix for Vin (Q)=0
    if(Vin.le.0) then
        WRITE(15,2685)0.d0
    else
        WRITE(15,2685)Vout/Vin
    endif
c--- rmc 04/20/03 --end of fix
    WRITE(15,*)'
    SMIN=GSIMASS*FWID/1000.d0
    WRITE(15,2700)SMIN
c--- rmc 04/20/03 --Fix for Vin (Q)=0
    if(Vin.le.0) then
        WRITE(15,2800)0.d0
    else
        WRITE(15,2800)GSIMASS*FWID/(Vin*1000.d0)
    endif
c--- rmc 04/20/03 --end of fix
    SMOUT=GSOMASS*FWID/1000.d0
    WRITE(15,2900)SMOUT
c--- rmc 04/20/03 --Fix for Vout=0
    if(Vout.le.0) then
        WRITE(15,3000)0.d0
    else
        WRITE(15,3000)GSOMASS*FWID/(Vout*1000.d0)
    endif
c--- rmc 04/20/03 --end of fix
    WRITE(15,3050)(GSIMASS-GSOMASS)*FWID/1000.d0
c--- rmc 04/20/03 --Fix for VIn=0
    if(Vout.le.0) then
        WRITE(15,3075)0.d0
    else
        WRITE(15,3075)SMOUT/SMIN
    endif
c--- rmc 04/20/03 --end of fix

WRITE(15,*)'
WRITE(15,3100)VLT/100.d0
WRITE(15,3200)XTOLD/100.d0
IF(NFUP.EQ.1) THEN
    WRITE(15,1850)
ELSEIF(YTOLD.EQ.H) THEN

```

```

        WRITE(15,1875)
ENDIF

c-(08/2008)-Water quality summary output file -----

! IWQPRO used instead of IWQ
!!WQPRO 1=Sabbag 2=FEMADR 3=tarse
!      IF(IWQ.GT.0) THEN
      IF(IWQPRO.EQ.1) THEN

          IF (SMIN.EQ.0.D0) THEN
              FPH=Vin*1000.D0/(VKD*0.001D0)
          ELSE
              FPH=Vin*1000.D0/(VKD*SMIN)
          ENDIF
          PDQ=VF/WAT_IN*100.D0
          PDSSED=TTE*100.D0
          DELTAP=24.79D0+.54D0*PDQ+.52*PDSSED-2.42D0*DLOG(FPH+1.D0)-.89D0*CCP
          IF (DELTAP.GT.100.D0.OR.PDQ.GE.100.) DELTAP=100.D0
          IF (PDQ.EQ.0.AND.PDSSED.EQ.0.) DELTAP=0.D0
          IF (DELTAP.LT.0.) DELTAP=0.D0
          WRITE(18,*)
          WRITE(18,*)Outputs for pesticide trapping (Sabbagh et al. 2009)'
          WRITE(18,*)-----'
          WRITE(18,4000)VIN
          WRITE(18,4100)SMIN
          WRITE(18,4200)FPH
          WRITE(18,4300)PDQ
          WRITE(18,4400)PDSSED
          WRITE(18,4450)100.D0*(1-Vout/Vin)
          WRITE(18,*)
          WRITE(18,4500)DELTAP
      END if

c-----Output message at end of program -----

      IF(ISCR.EQ.0) THEN
WRITE(*,*)
WRITE(*,*)...FINISHED...','VFSMOD v5.0.0 03/2010'
WRITE(*,*)
ENDIF

150  FORMAT('Volume from outflow = ', E14.4,' m3')
200  FORMAT('Volume from i_e   = ', E14.4,' m3',F14.2,'%')
300  FORMAT('Volume from up-field= ', E14.4,' m3')
400  FORMAT('Volume infiltrated = ', E14.4,' m3')
500  FORMAT(F8.2,3E12.4,I6)
600  FORMAT('Volume from rainfall= ', E14.4,' m3')
700  FORMAT('Time to beginning   = ', E14.4,' s')
800  FORMAT('Time and q at peak = ', E14.4,' s',E14.4,' m3/s')
900  FORMAT('Time to end runoff  = ', E14.4,' s')
1010 FORMAT('Trapping efficiency =      ', F5.1,'%')
1100 FORMAT('Sediment inflow   = ', E14.4,' g/cm',E14.4,' g')
1200 FORMAT('Sediment outflow  = ', E14.4,' g/cm',E14.4,' g')
1250 FORMAT('Sediment deposition :')
1300 FORMAT(8x,'- Sediment wedge depth,  Y(t) =',F7.2,'cm')
1400 FORMAT(8x,'- Sediment wedge length, X2(t) =',F7.2,'cm')
1500 FORMAT(8x,'- Effective filter length,L(t) =',F7.2,'cm')
1600 FORMAT(8x,'- Sediment tail at field, X1(t) =',F7.2,'cm')
1700 FORMAT(8x,'- Sediment depth in low section =',F7.2,'cm')
1800 FORMAT(8x,'- Rough sediment balance error =',F7.2,'%')
1825 FORMAT(8x,'- Rough water balance error =',F7.2,'%')
1850 format(/,66('*'),/* WARNING: Strip filled up!,37x,**,
& /,66('*'))
1875 format(/,67('*'),/* WARNING: Top of vegetation reached',
& ' - trapezoidal wedge started *,/,67('*'))
1900 FORMAT(1x,F8.2,' m^2 = Source Area (input)')
2000 FORMAT(1x,F8.2,' m = Source Flow Length (input)')
2100 FORMAT(1x,F8.2,' m = Source Area Width (input)')
2200 FORMAT(1x,F8.2,' m = Filter Strip Length (input)')

```

```

2225  FORMAT(1x,F8.2,' m = Filter Strip Width (input)')
2250  FORMAT(1x,F8.3,' = Mean Filter Mannings Roughness (input)')
2300  FORMAT(1x,F8.2,' % = ',
1     'Ratio of Filter Length to Source Flow Length')
2400  FORMAT(1x,F8.3,' mm = Total Rainfall')
2450  FORMAT(1x,F8.3,' m3 = Total Rainfall on Filter')
2500  FORMAT(1x,F8.3,' mm = Total Runoff from Source (mm depth over',
&     ' Source Area)')
2550  FORMAT(1x,F8.3,' m3 = Total Runoff from Source')
2600  FORMAT(1x,F8.3,' mm = Total Runoff out from Filter (mm depth',
&     ' over Source+Filter)')
2650  FORMAT(1x,F8.3,' m3 = Total Runoff out from Filter')
2675  FORMAT(1x,F8.3,' m3 = Total Infiltration in Filter')
2685  FORMAT(1x,F8.3,' = Runoff Delivery Ratio')
2700  FORMAT(F10.3,' kg = Mass Sediment Input to Filter')
2800  FORMAT(F10.3,' g/L= Concentration Sediment in Runoff from',
&     ' source Area')
2900  FORMAT(F10.3,' kg = Mass Sediment Output from Filter')
3000  FORMAT(F10.3,' g/L= Concentration Sediment in Runoff exiting',
&     ' the Filter')
3050  FORMAT(F10.3,' kg = Mass Sediment retained in Filter')
3075  FORMAT(2x,F8.3,' = Sediment Delivery Ratio')
3100  FORMAT(1x,F8.2,' m = Effective Filter Length')
3200  FORMAT(1x,F8.2,' m = Wedge Distance')
4000  FORMAT(F10.3,' m3 = Runoff inflow')
4100  FORMAT(F10.3,' Kg = Sediment inflow')
4200  FORMAT(F10.3,' = Phase distribution, Fph')
4300  FORMAT(F10.3,' % = Infiltration (dQ)')
4400  FORMAT(F10.3,' % = Sediment reduction (dE)')
4450  FORMAT(F10.3,' % = Runoff inflow reduction')
4500  FORMAT(F10.3,' % = Pesticide reduction')

```

```

RETURN
END

```

SUBROUTINE QUADtrt

```

ICCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
IC THE SUBROUTINE QUAD DEFINES THE VALUES OF THE PARAMETERS
IC REQUIRED FOR THE NUMERICAL INTEGRATION OF ELEMENT MATRICES
IC AND VECTORS. THESE DATA ARE PROBLEM INDEPENT AND ARE GIVEN
IC OVER THE INTERVAL [-1,1].
IC CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  ! Dimension Xltrt(i,i),Wtrt(i,i)
  COMMON/CINTtrt/Xltrt(4,4),Wtrt(4,4)

IC Gaussian Quadrature of order 1
  Xltrt(1,1) = 0.D0
  Wtrt(1,1) = 2.D0
IC Gaussian Quadrature of order 2
  Xltrt(1,2) = -1.D0/DSQRT(3.D0)
  Xltrt(2,2) = -Xltrt(1,2)
  Wtrt(1,2) = 1.D0
  Wtrt(2,2) = Wtrt(1,2)
IC Gaussian Quadrature of order 3
  Xltrt(1,3) = -DSQRT(3.D0/5.D0)
  Xltrt(2,3) = 0.D0
  Xltrt(3,3) = -Xltrt(1,3)
  Wtrt(1,3) = 5.D0/9.D0
  Wtrt(2,3) = 8.D0/9.D0
  Wtrt(3,3) = Wtrt(1,3)
IC Gaussian Quadrature of order 4
  Xltrt(1,4) = -0.8611363116D0
  Xltrt(2,4) = -0.3399810436D0
  Xltrt(3,4) = -Xltrt(2,4)
  Xltrt(4,4) = -Xltrt(1,4)

```


COMMON/RSE2/STAB2,STAB3,STAB4,STAB5,STAB6,ISPLIT
COMMON/RSE3/Atrt,Atrt2,Atr3,BMtrt,BMtrt2,BMtrt3,Btrt,Btrt2,Btrt3
CHARACTER*75 LISFIL(13)

DIMENSION A(MAXEQN,MAXBND),BM(MAXEQN,MAXBND) ,B(MAXEQN)
DIMENSION X(MAXEQN) ,X0(MAXEQN),C2(50),C1(50),
DISLtrt(5),DISMtrt(3)
DIMENSION STAB2(MAXEQN),STAB3(MAXEQN),STAB4(MAXEQN)
DIMENSION STAB5(MAXEQN), STAB6(MAXEQN)
DIMENSION Atrt(MAXEQN,MAXBND),BMtrt(MAXEQN,MAXBND) ,Btrt(MAXEQN)
DIMENSION Atrt2(MAXEQN,MAXBND),BMtrt2(MAXEQN,MAXBND),Btrt2(MAXEQN)
DIMENSION Atrt3(MAXEQN,MAXBND),BMtrt3(MAXEQN,MAXBND),Btrt3(MAXEQN)
Character(len=120), **Dimension**(50) :: varname
CHARACTER (len=120) :: XMLinput1,XMLinput
CHARACTER (len=120) :: XMLoutput
CHARACTER (len=120) :: XMLreac_set
integer(kind=4) :: WQflag,nmob,nstab,npar,tot,m,nvarX

Character (len=120) :: filename
CHARACTER*1 mm

OPEN(17,FILE=LISFIL(12))

```
!Opens and read input file .iwq for RSE
!  open (unit=33, file=filename)
  read(17,*) WQflag !WQflag
! Read XML input file, XML outout file to check indexes, react set to be used in XML input file
  read(17,*) XMLinput, XMLoutput, XMLreac_set
! Read mobile variables
  read(17,*) nmob,(varname(i),C2(i),DISLtrt(i),DISMtrt(i),i=1,nmob)
  if (nmob.eq.1) then
    CONC1=C2(1)
    DISL=DISLtrt(1)
    DISM=DISMtrt(1)
  ELSE
!NEED TO ADD AN OPTION FOR MORE MOBILE TRANSPORT PARAMETERS for more than
! one mobile component
  endif
! Read stabile variables
  read(17,*) nstab, (varname(j),C2(j),j=(nmob+1),(nmob+nstab))
  nvarX=nmob+nstab
  j=nmob+nstab
  n=nmob+nstab
  IF (nstab.eq.1) then
    DO 10 l=1,MAXEQN
      STAB2(l)=C2(2)
10    CONTINUE
  end IF
  IF (nstab.eq.2) then
    DO 20 l=1,MAXEQN
      STAB2(l)=C2(2)
      STAB3(l)=C2(3)
20    CONTINUE
  END IF
  IF (nstab.eq.3) then
    DO 30 l=1,MAXEQN
      STAB2(l)=C2(2)
      STAB3(l)=C2(3)
      STAB4(l)=C2(4)
30    CONTINUE
  END IF
  IF (nstab.eq.4) then
    DO 40 l=1,MAXEQN
      STAB2(l)=C2(2)
      STAB3(l)=C2(3)
      STAB4(l)=C2(4)
      STAB5(l)=C2(5)
40    CONTINUE
  END IF
  IF (nstab.eq.5) then
```

```

DO 50 I=1,MAXEQN
  STAB2(I)=C2(2)
  STAB3(I)=C2(3)
  STAB4(I)=C2(4)
  STAB5(I)=C2(5)
  STAB6(I)=C2(6)
50 CONTINUE
END IF
! Read parameter to be used (usually declared to be used in the set of equations)
k=j+27+6+1
j=k
!(19 intrinsic + 8 dispersion-diffusion parameters = 27; +6 for:
! TSED,FSSED,CSED,SEDFVS,INFRATE,HRO)
read(17,*) npar, (varname(k),C2(k),k=j,(j+npar-1)) !
! Read intrinsic values of depth, x_vel_ol, time_step, area if m="1"
READ(17,*)mm
  m=INDEX(mm,'1')
  IF(m.EQ.1) then
    read(17,*) varname(n+2),C2(n+2),varname(n+16),C2(n+16),
& varname(n+20),C2(n+20),varname(n+1),C2(n+1)
    dtRSE=C2(n+20)
  end if
tot=j+npar-1
C1=C2 !Return vector to the hydrodynamic driving program
!ntoto Returns the total number of indexes (Estimated. To confirm order, check XML output)
ntot=tot
close(17)
end

```

Subroutine runRSE(M,WW,VV,rk_order1,time_step1,input_filename1C,output_filename1C,reaction_set1C,init1)

```

use IFPORT
implicit none
! print *, 'Test 1: ', M
Real(kind=8), Dimension(50) :: WW
integer(kind=4) :: M,VV
Integer(kind=4) :: a, b, init1
Integer(kind=4) :: nvals,varnum
Integer(kind=4) :: rk_order,rk_order1 ! Either 2 or 4
Real(kind=8) :: time_step, time_step1, temp_dt
Real(kind=8), Dimension(M) :: vars
CHARACTER (len=120) :: input_filename,input_filename1
CHARACTER (len=120) :: output_filename,output_filename1
CHARACTER (len=120) :: reaction_set, reaction_set1
integer*1, Dimension (50):: input_filename1C, output_filename1C, reaction_set1C
integer*1, Dimension (50):: input_filename1A, output_filename1A, reaction_set1A

Interface to Subroutine Initialize ( input_xml, output_xml, rname )
  !DEC$ Attributes C, DLLIMPORT, alias: "_Initialize" :: Initialize
  integer*1, Dimension (50):: input_xml, output_xml, rname
  !new input files as arrays of chars instead of strings
  !DEC$ Attributes REFERENCE :: input_xml
  !DEC$ Attributes REFERENCE :: output_xml
  !DEC$ Attributes REFERENCE :: rname
END
Interface to Subroutine PreSolve ( num_var, vars )
  !DEC$ Attributes C, DLLIMPORT, alias: "_PreSolve" :: PreSolve
  Integer(kind=4) :: num_var
  Real(kind=8), Dimension(num_var) :: vars
End
Interface to Subroutine PostSolve ( num_var, vars )
  !DEC$ Attributes C, DLLIMPORT, alias: "_PostSolve" :: PostSolve
  Integer(kind=4) :: num_var
  Real(kind=8), Dimension(num_var) :: vars
End
Interface to Subroutine RKSolve ( time_step, order, num_var, vars )

```



```

DIMENSION TSED(MAXEQN),FSED(MAXEQN),CSED(MAXEQN),SEDEVFS(MAXEQN)
DIMENSION XPOINTS(3),NODEX(4)

! Calculation for Sed Conc in runoff on triangular wedgeZone
IF (NODEX(4).eq.1) then
! Sed's runoff concentration in wedge slope (X2 zone)
  IF (NODEX(2).gt.1) then
    SLOPEW=(GS2-GSI)/(NODEX(2)-1)
    DO 10 i=1, nodex(2)
      TSED(i)=(SLOPEW*(i-1)+GSI)*FWID/Q0(i)
      CSED(i)=(1-FI)*TSED(i)
      FSED(i)=TSED(i)-CSED(i)
10  CONTINUE
  ELSE
! This options means no wedge section developed
    TSED(1)=(GSI)*FWID/Q0(i)
    CSED(1)=COARSE*TSED(1)
    FSED(1)=(1-COARSE)*TSED(1)
  END IF

! Calculation for Sed Conc in runoff suspended load zone
  IF (GS2.GT.0) then
    SLOPELT=(GSO-GS2)/(N-NODEX(2))
    IF (SLOPELT.gt.0) then
! when slopel>0 GS2 & GSO are different, the calculate
! sediment concentration in runoff by linear decrement
      DO 30 i=NODEX(2), N
        if (i.eq.1) then
          TSED(1)=GS2*FWID/Q0(i)
          CSED(i)=(1-FI)*TSED(i)
          FSED(i)=TSED(i)-CSED(i)
        else
          TSED(i)=(SLOPELT*(i-NODEX(2))+GS2)*FWID/Q0(i)
          CSED(i)=(1-FI)*TSED(i)
          FSED(i)=TSED(i)-CSED(i)
        end if
30  CONTINUE
      end if
    IF (SLOPELT.eq.0) then
! when slopel=0 GS2=GSO, then concentration is constant
      DO 35 i=NODEX(2), N
        TSED(1)=GS2*FWID/Q0(i)
        CSED(i)=(1-FI)*TSED(i)
        FSED(i)=TSED(i)-CSED(i)
35  CONTINUE
      end if
    end if
  END IF

! Trapezoidal wedge developed
! No change in conc. for Zone(A) of wedge
  IF ((NODEX(4).gt.1).and.(NODEX(4).lt.N)) then
    DO 40 i=1,NODEX(4)
      TSED(i)=GSI*FWID/Q0(i)
      FSED(i)=(1-COARSE)*TSED(i)
      CSED(i)=COARSE*TSED(i)
40  CONTINUE
! Sed's runoff Conc in zone (B) of wedge
    SLOPEW=(GS2-GSI)/(NODEX(2)-NODEX(4))
    DO 50 i=NODEX(4), nodex(2)
      TSED(i)=(SLOPEW*(i-NODEX(4))+GSI)*FWID/Q0(i)
      CSED(i)=(1-FI)*TSED(i)
      FSED(i)=TSED(i)-CSED(i)
50  CONTINUE
! Sed's runoff concentration in Suspended Load Zone
    DO 60 i=NODEX(2), N
      TSED(i)=(SLOPELT*(i-NODEX(2))+GS2)*FWID/Q0(i)
      CSED(i)=(1-FI)*TSED(i)
      FSED(i)=TSED(i)-CSED(i)

```

```

60 CONTINUE
! end if
END IF

! When the filter is full, GSO=GSI
IF (NODEX(4).eq.N) then
DO 70 i=1, N
TSED(i)=GSI*FWID/Q0(i)
FSED(i)=(1-COARSE)*TSED(i)
CSED(i)=COARSE*TSED(i)
70 CONTINUE
END IF

!----- Deposited sediment concentration on VFS -----
! sediment concentration in Suspended Sediment Zone
VOLSEDLT=FWID*VLT*DEP
VOLSEDLT2=VOLSEDLT*POR
ZMASSLT=VOLSEDLT2*PART(3)

DO 80 i=NODEX(2), N
SEDFVS(i)=ZMASSLT/VOLSEDLT*1E6
! 1E6 transform g/cm3 to g/m3
80 CONTINUE

! IF no wedge zone, then all is taken as suspended sediment zone
if (YT.eq.0) then
VOLSEDLT=FWID*VLCM*DEP
VOLSEDLT2=VOLSEDLT*POR
ZMASSLT=VOLSEDLT2*PART(3)
DO 90 i=1, N
SEDFVS(i)=ZMASSLT/VOLSEDLT*1E6
! 1E6 transform g/cm3 to g/m3
90 CONTINUE
end if

! Time step in cm
DXcm=VX*100

! Sed's runoff concentration in wedge slope (X2 zone)

IF (YT.gt.0) then
IF (NODEX(4).eq.1) then

IF (NODEX(2).gt.1) then
SLOPEW=-YT/XPOINTS(2)
DO 100 i=1, nodex(2)
YTi=SLOPEW*(i*DXcm)+YT
VOLSEDLT=FWID*DXcm*YTi
VOLSEDLT2=VOLSEDLT*POR
ZMASSLT=VOLSEDLT2*PART(3)
SEDFVS(i)=ZMASSLT/VOLSEDLT*1E6
100 CONTINUE
ELSE
! This options means no wedge section developed
! Nodex(1)(2) and (4) are the same (node 1)
VOLSEDLT=FWID*DXcm*YT
VOLSEDLT2=VOLSEDLT*POR
ZMASSLT=VOLSEDLT2*PART(3)
SEDFVS(1)=ZMASSLT/VOLSEDLT*1E6
END IF

END IF
END IF

! This option accounts for a trapezoidal wedge
! Sediemnt concentration constant in wedge (Section A)
IF ((NODEX(4).gt.1).and.(NODEX(4).lt.N)) then
DO 110 i=1,NODEX(4)
VOLSEDLT=FWID*DXcm*YT
VOLSEDLT2=VOLSEDLT*POR

```

```

      ZMASSLT=VOLSEDLT2*PART(3)
      SEDVFS(i)=ZMASSLT/VOLSEDLT*1E6
110  CONTINUE
! Sed's runoff Conc in zone (B) of wedge
      SLOPEW=-YT/(NODEX(2)*DXcm-NODEX(4)*DXcm)
      IF (NODEX(2)-NODEX(4).gt.0) then
        DO 120 i=NODEX(4), nodex(2)
          YTi=SLOPEW*(i*DXcm)+YT
          VOLSEDLT=FWID*DXcm*YTi
          VOLSEDLT2=VOLSEDLT*POR
          ZMASSLT=VOLSEDLT2*PART(3)
          SEDVFS(i)=ZMASSLT/VOLSEDLT*1E6
120  CONTINUE
      end if
      END IF

! When the filter is full, DEP=YT
      IF (NODEX(4).eq.N) then
        VOLSEDLT=FWID*VLT*YT
        VOLSEDLT2=VOLSEDLT*POR
        ZMASSLT=VOLSEDLT2*PART(3)
        DO 130 i=NODEX(2), N
          SEDVFS(i)=ZMASSLT/VOLSEDLT*1E6
! 1E6 transform g/cm3 to g/m3
130  CONTINUE
      END IF
      return
      end

```

```

      SUBROUTINE SHAPEtrt(XI,N,PSI,DPSI)
!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
!C SUBROUTINE SHAPE CALCULATES THE VALUES OF THE SHAPE
!C FUNCTION PSI AND THEIR DERIVATIVES DPSI WITH RESPECT TO
!C THE MASTER ELEMENT COORDINATES AT A SPECIFIED VALUE OF XI.
!C
!C ANY TYPICAL ELEMENT = [X1,Xk+1] CONSISTING OF k+1 NODES
!C X1, ..., Xk+1 IS ALWAYS NORMALIZED INTO THE MASTER
!C ELEMENT = [-1,1] BY THE TRANSFORMATION OVER A TYPICAL
!C ELEMENT [X1,Xk+1] THERE EXIST k+1 ELEMENT SHAPE FUNCTIONS
!C PSI, EACH IS A POLYNOMIAL OF DEGREE k.
!C
!C   XI: THE MASTER COORDINATE OF THE POINT AT WHICH
!C   VALUES OF PSI AND D PSI ARE DESIRED
!C   N : NUMBER OF NODES IN THE ELEMENT
!C   (AND HENCE NUMBER OF SHAPE FUNCTIONS)
!C PSI(I) : THE I-TH SHAPE FUNCTION AT XI
!C DPSI(I) : THE DERIVATIVE OF THE I-TH SHAPE FUNCTION AT XI
!CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PSI(4),DPSI(4)
      IF (N.LT.2.OR.N.GT.4) GO TO 99
      GO TO (99,10,20,30) N

!C Linear Basis functions -----
10  PSI(1) = .5D0*(1.D0-XI)
     PSI(2) = .5D0*(1.D0+XI)
     DPSI(1) = -.5D0
     DPSI(2) = .5D0
     RETURN

!C Quadratic basis functions -----
20  PSI(1) = XI*(XI-1.D0)*0.5D0
     PSI(2) = 1.D0-XI**2.D0
     PSI(3) = XI*(XI+1.D0)*0.5D0
     DPSI(1) = XI-0.5D0
     DPSI(2) = -2.D0*XI
     DPSI(3) = XI+0.5D0

```

RETURN

!C Cubic shape function-----

```

30  PSI(1) = 9.D0/16.D0*(1.D0/9.D0-XI**2.D0)*(XI-1.D0)
    PSI(2) = 27.D0/16.D0*(1.D0-XI**2.D0)*(1.D0/3.D0-XI)
    PSI(3) = 27.D0/16.D0*(1.D0-XI**2.D0)*(1.D0/3.D0+XI)
    PSI(4) = -9.D0/16.D0*(1.D0/9.D0-XI**2.D0)*(1.D0+XI)
    DP(1) = -9.D0/16.D0*(3.D0*XI**2-2.D0*XI-1.D0/9.D0)
    DP(2) = 27.D0/16.D0*(3.D0*XI**2-2.D0/3.D0*XI-1.D0)
    DP(3) = 27.D0/16.D0*(-3.D0*XI**2-2.D0/3.D0*XI+1.D0)
    DP(4) = -9.D0/16.D0*(-3.D0*XI**2-2.D0*XI+1.D0/9.D0)

```

RETURN

99 **WRITE**(6,*) 'ERROR IN CALLING TO SHAPE (NPOL OUT OF RANGE)=',N

STOP

END

SUBROUTINE SOLVE(A,B,X,N,NBAND)

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C      SOLVE THE TRANSFORMED MATRIX A USING A BACKWARD AND FORWARD SUBSTITUTION C
C      SUCH:   [A] {x} = {b}
C      Since  [A] = [L].[U] then [L][U]{x} = [L]([U]{x}) = [L]{y} = {b}
C      solving [L]{y} = {b} (forward substitution)
C      [U]{x} = {y} (backward substitution)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

```

PARAMETER (MAXEQN=1001,MAXBND=40)

IMPLICIT DOUBLE PRECISION (A-H, O-Z)

DIMENSION A(MAXEQN,MAXBND), B(MAXEQN), X(MAXEQN)

NDIAG = (NBAND/2)+1

NMAX = NBAND-NDIAG

M = N -1

DO 10 I = 1,M

NA = NMAX

IF(NA .GT. N -I) NA = N -I

DO 10 J = 1,NA

B(I+J) = B(I+J)+A(I+J,NDIAG-J)*B(I)

10 **CONTINUE**

X(N) = B(N)/A(N,NDIAG)

DO 20 J = M,1,-1

NA = NMAX

IF(NA .GT. N -J) NA = N -J

DO 30 K = 1,NA

B(J) = B(J)-X(J+K)*A(J,NDIAG+K)

30 **CONTINUE**

X(J) = B(J)/A(J,NDIAG)

20 **CONTINUE**

RETURN

END

SUBROUTINE WQSUB(TIME,NBAND,N,LISFIL,iTRTcount,Lcount,FPI,rainWQ)

```

!from vfstmod      call WQSUB(TIME,NBAND,N,LISFIL,iTRTcount,Lcount,rainWQ)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C Water quality component skeleton          C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      PARAMETER (MAXEQN=1001,MAXBND=40)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      CHARACTER*75 LISFIL(13)
      COMMON/WQ1/VKD,CCP,IWQPRO
! call pesticides, femadr or tarse based on IWQPRO (2 or 3)
      if (IWQPRO.GT.1) call FEMADR(iTRTcount,LCOUNT,TIME,LISFIL,
&          NBAND,N,FPI,rainWQ)
      RETURN
      END

```

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BIOGRAPHICAL SKETCH

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