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Modeling watershed-scale solute transport using an integrated, process-based hydrologic model with applications to bacterial fate and transport

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SUMMARY

Distributed hydrologic models that simulate fate and transport processes at sub-daily timescales are useful tools for estimating pollutant loads exported from watersheds to lakes and oceans downstream. There has been considerable interest in the application of integrated process-based hydrologic models in recent years. While the models have been applied to address questions of water quantity and to better understand linkages between hydrology and land surface processes, routine applications of these models to address water quality issues are currently limited. In this paper, we first describe a general process-based watershed-scale solute transport modeling framework, based on an operator splitting strategy and a Lagrangian particle transport method combined with dispersion and reactions. The transport and the hydrologic modules are tightly coupled and the interactions among different hydrologic components are explicitly modeled. We test transport modules using data from plot-scale experiments and available analytical solutions for different hydrologic domains. The numerical solutions are also compared with an analytical solution for groundwater transit times with interactions between surface and subsurface flows. Finally, we demonstrate the application of the model to simulate bacterial fate and transport in the Red Cedar River watershed in Michigan and test hypotheses about sources and transport pathways. The watershed bacterial fate and transport model is expected to be useful for making near real-time predictions at marine and freshwater beaches.

1. Introduction

The ability to quantify fluxes of nutrients, bacteria, viruses and other contaminants exported from watersheds to downstream receiving water bodies such as lakes and oceans is important for managing coastal resources (e.g., to generate timely predictions of water quality for beach closures, e.g., Ge et al., 2012a,b) and to understand and assess threats to human and ecosystem health. In the Great Lakes region of North America, for example, increased beach closures due to microbiological pollution, eutrophication and harmful algal blooms and drinking water related issues continue to be causes for concern highlighting the need for well-tested and reliable transport models. Integrated process-based hydrologic models, which are based on the conservation principles of mass, momentum and energy, are useful tools for making accurate predictions and have the potential to offer insights into the fundamental transport processes at the watershed scale. A number of such watershed models have been developed in the last few decades including, for example, CATHY (Weill et al., 2011), InHM (VanderKwaak, 1999), OpenGeoSys (Kolditz et al., 2012), ParFlow (Kollet and Maxwell, 2006), PAWS (Shen and Phanikumar, 2010), tRIBS (Ivanov et al., 2004) and Wash123 (Yeh et al., 2011). Although a majority of these models have the ability to simulate transport processes, the routine application of process-based hydrologic models to address water quality issues is currently still limited.

The assessment and management of non-point sources of pollution (e.g., microbial pollution) is an issue of great interest. *Escherichia coli* (*E. coli*) is a commonly used fecal indicator organism in freshwaters. Prior research has shown that *E. coli* densities are correlated with swimming-associated gastroenteritis (Prüss, 1998). Models such as MWASTE (Moore et al., 1989), COLI (Walker et al., 1990) and SEDMOD (Fraser et al., 1998) have been developed to simulate landscape microbial pollution processes. These models successfully simulate the manure-borne bacteria

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releasing process and the transport of bacteria through runoff; however, the die-off due to solar radiation and other environmental factors was not considered, and there was no interaction among different hydrologic components in these models. There are models incorporating both landscape and in-stream microbial processes, for example, the Soil and Water Assessment Tool (SWAT) (Frey et al., 2013), a watershed model developed by Tian et al. (2002), a modified SWAT model (Cho et al., 2012), which considered solar radiation associated bacterial die-off, and a coastal watershed fecal coliform fate and transport model based on HSPF (Hydrologic Simulation Program Fortran, Rolle et al., 2012). These models tend to use conceptual representations of the groundwater and vadose zone compartments, ignoring the complexity of the flow in the subsurface domain. The subsurface flow is an integral component of the hydrologic cycle and in shallow water table conditions groundwater controls soil moisture and provides sources of water for evapotranspiration (ET) (Shen and Phanikumar, 2010). Therefore, the subsurface flow domain should be fully considered while developing a general framework for the solute transport problem even if the subsurface contribution is not important for certain types of pollutants.

A process-based, watershed-scale reactive transport modeling framework is developed in this work to quantify the fluxes of conservative and reactive solutes exported from watersheds. The distributed hydrologic model PAWS (Process-based Adaptive Watershed Simulator, Shen and Phanikumar, 2010; Shen et al., 2013; Niu et al., 2014) was used to simulate integrated hydrology, including flows in channel networks, overland flow, and subsurface flows and interactions between different domains. The computational efficiency of the PAWS model allows for long-term, large-scale simulations and makes it possible to simulate transport in large watersheds. An operator-splitting strategy (e.g., Phanikumar and McGuire, 2004) combined with a Lagrangian particle transport modeling approach (e.g., de Rooij et al., 2013) with reactions to describe transport in different hydrologic units was applied. Due to the complexity of the processes involved, extensive model testing against analytical solutions for different hydrologic domains is a necessary first step before the performance of the integrated model can be fully evaluated. Such detailed testing provides a way to ascertain the sources of error when model inter-comparison exercises are conducted (e.g., Maxwell et al., 2014). In the present paper, the algorithms were tested using available analytical solutions and data from plot-scale experiments before applying the bacterial fate and transport model to describe monitoring data from the Red Cedar River watershed in the Great Lakes region. Future papers will describe additional model testing (especially interactions between the groundwater and surface water domains) as well as the development and application of additional transport modules (e.g., carbon, nitrogen and phosphorus cycles).

2. Methods

2.1. 2D overland flow transport

A commonly accepted approximation of the St. Venant equations for overland flow is the kinematic wave equation (Singh, 1996) which can be expressed as:

$$\frac{\partial h}{\partial t}+\frac{\partial(uh)}{\partial x}+\frac{\partial(vh)}{\partial y}=S \tag{1}$$

where h is the overland flow water depth [L], u, v are the x- and y-direction water velocities [LT^{-1}], S is either a source term to represent precipitation or exfiltration from the subsurface, or a sink term to represent infiltration or evaporation. The solute transport equation for overland flow can be expressed in a conservative form in terms of the solute flux (Deng et al., 2006) as:

$$\frac{\partial(C_o h)}{\partial t}+\frac{\partial(C_o uh)}{\partial x}+\frac{\partial(C_o vh)}{\partial y}=\frac{\partial}{\partial x}\left(hD_x\frac{\partial C_o}{\partial x}\right)+\frac{\partial}{\partial y}\left(hD_y\frac{\partial C_o}{\partial y}\right)+rD_m(C_s-C_o)-kC_o h \tag{2}$$

where the subscript o denotes overland flow, C_o is the cross-sectionally averaged solute concentration [ML^{-3}] or the mass of solute per unit volume of runoff; C_S represents the solute concentration in the soil mixing zone; r is a mass transfer coefficient [T^{-1}]; D_m is the mixing zone thickness [L] which is proportional to flow depth; k is the decay coefficient [T^{-1}]; D_x and D_y are the x- and y-direction diffusion coefficients [L^2T^{-1}]. Eq. (2) can be fully expanded and rearranged as below:

$$C_o\left(\frac{\partial h}{\partial t}+\frac{\partial(uh)}{\partial x}+\frac{\partial(vh)}{\partial y}\right)+h\left(\frac{\partial C_o}{\partial t}+u\frac{\partial C_o}{\partial x}+v\frac{\partial C_o}{\partial y}\right)=h\left(D_x\frac{\partial^2 C_o}{\partial x^2}+D_y\frac{\partial^2 C_o}{\partial y^2}\right)+D_x\frac{\partial h}{\partial x}\frac{\partial C_o}{\partial x}+D_y\frac{\partial h}{\partial y}\frac{\partial C_o}{\partial y}+rD_m(C_s-C_o)-kC_o h \tag{3}$$

Using the kinematic wave approximation which ignores the pressure gradient terms, we have $\partial h/\partial x = 0$ and $\partial h/\partial y = 0$. Substituting Eqs. (1) into (3) and dividing both sides of the above equation by the flow depth h gives the following equation:

$$\frac{\partial C_o}{\partial t}+u\frac{\partial C_o}{\partial x}+v\frac{\partial C_o}{\partial y}=D_x\frac{\partial^2 C_o}{\partial x^2}+D_y\frac{\partial^2 C_o}{\partial y^2}+\frac{rD_m}{h}(C_s-C_o)-\left(\frac{S}{h}+k\right)C_o \tag{4}$$

2.2. Channel flow, the river network and river junctions

The one-dimensional channel transport equation used in the present work appears as shown below (see, for example, Gunduz, 2004):

$$\frac{\partial(C_r A)}{\partial t}+\frac{\partial}{\partial x}(vAC_r)-\frac{\partial}{\partial x}\left(AD_L\frac{\partial C_r}{\partial x}\right)+kC_r A-q_L C_L+n_{sed}D_{sed}\frac{C_g-C_r}{m_r}w_r-q_o C_o=0 \tag{5}$$

where C_r is the solute concentration within the river channel, C_L and C_o are concentrations associated with lateral seepage and overland flows respectively, q_L and q_o are lateral seepage and overland flows per channel length [$L^3T^{-1}L^{-1}$] (considered positive for inflow), A is the cross-sectional flow area [L^2], D_L is the longitudinal dispersion coefficient in the channel [L^2T^{-1}], D_{sed} is vertical dispersion coefficient [L^2T^{-1}] in the sediment layer, n_{sed} is porosity of the sediment layer (dimensionless), C_g is solute concentration associated with groundwater flow, m_r is thickness of the sediment layer [L], and w_r is river wetted perimeter [L].

Initial solute concentrations need to be specified along the one-dimensional channel domain: $C_r(x, 0) = C_{r0}(x)$, where C_{r0} is the initial concentration distribution along the channel network. Concentration boundary conditions in the form of Dirichlet, Neumann or mixed type can be specified at the external ends of the domain depending on whether a specified concentration or diffusional or total mass flux is being specified.

In addition, internal boundary conditions may need to be specified when two or more channels join to form a junction. While handling river junctions, the change in mass storage within a junction is assumed to be negligible compared to the change in mass within the channel. Furthermore, the continuity of concentration at junctions guarantees that all the concentrations must be equal at junctions. Eq. (5) is first solved by an advection step using