Mathematical model development for non-point source in-stream pollutant transport

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Abstract: Non-point source pollution is a primary cause for concern globally. Various models have been developed to tackle this situation with much emphasis placed on best management practices. This practice has, however, proven to be insufficient to solve the NPS pollution situation. Existing non-point source models are watershed--based and complicated both in operation, parameter estimation and data requirements. A non-point source model is proposed using the concept of the Hybrid Cells in Series model. The model is a three-parameter model made up of three zones, which describes pure advection through time delay in a plug zone, with combined advection and dispersion occurring when the other two zones are considered as thoroughly mixed. The proposed model is tested using synthetic data and field data from the Snake River, Colorado, USA, obtained from literature. Simulations were performed at four sample points; two from the tracer injection point along the Snake River before a confluence and two further downstream after the confluence. A regression analysis was carried out to determine the model's capability to simulate pollutant transport for the four sampling points. The coefficients of determination are 0.98, 0.94, 0.84 and 0.97 while the standard error for each reach is 2.28E-2, 2.70E-2, 2.32E-2 and 9.35E-3 respectively. The results show good agreement between the measured and the simulated data. The response of the C-t profiles produced by the proposed model for both synthetic and field data demonstrates its ability to effectively simulate pollutant transport in natural rivers subject to non-point source pollution.

Introduction

The release of pollutants in water environments through overland flows is on an alarming increase (Wang et al. 2013, Hu and Huang 2014). Pollutants originate from agricultural runoff, informal settlements, and urban areas, henceforth, Non-Point Sources (NPS), and discharge into receiving waters which impacts the eco-environment and humans negatively (Wen et al. 2017, Bojarczuk et al. 2019). This pollution process is complex involving diverse pollutant types, originating from varying sources. Hence, NPS pollution is considered a significant environmental and water quality problem globally (Shen et al. 2011, Fu et al. 2013, Wiatkowski and Wiatkowska 2019). Studies on NPS pollution control focus primarily on best management practices (BMP). Though BMP limits NPS pollution, it does not prevent the entry of NPS pollutants in rivers (Voza et al. 2015). NPS pollutants are distributed along the river channel from diffuse sources. Consequently, though the amounts deposited at any specific point of a river may be small due to BMP, the cumulative mass loading is substantial with its impact extending downstream (Runkel and Bencala 1995). Thus, a good understanding of the spatial and temporal characteristics of NPS pollution is required for effective control (Huang and Hong 2010, Chen et al. 2013).

Modeling is an effective mechanism for quantifying the spatio-temporal characteristics of NPS pollution. It simplifies the intricate processes of generation and transformations associated with this pollutant type (Wang et al. 2013). Attempts to address NPS pollution led to the development of several models at different scales (Ongley et al. 2010, Lam et al. 2010, Zhang et al. 2012, Olowe and Kumarasamy 2018). Models such as AnnAGNPS, an annualized version of AGNPS, SWAT and HSPF are some of the widely used NPS models. A significant drawback with these models is the intricacy in their operations, which require high levels of expertise, large data sets, exhaustive parameter estimation processes, extensive calibration and validation processes (Huang and Hong 2010, Zhang and Huang 2011, Shen et al. 2011, Chen et al. 2013, Ouyang et al. 2016). Several researchers (Borah and Bera 2004, Ongley et al. 2010, Li et al. 2014, Adu and Kumarasamy 2018) have evaluated NPS pollution in watersheds using these models. Diaz-Ramirez et al. (2011) simulated the hydrological processes in selected watersheds in Alabama, Mississippi, and Puerto Rico using HSPF. Chahor et al. (2014) assessed the suitability of AnnAGNPS to predict runoff and sediment yield in a small Mediterranean agricultural watershed in Spain. Lam et al. (2010) applied SWAT in modeling point and diffuse pollution of nitrate in Kielstau catchment area, North

Germany. These models are predominantly used for evaluation of NPS pollution with relation to rainfall-runoff processes, soil erosion, sediment transport, pollutant source identification and migration within catchments (Chen et al. 2013, Ouyang et al. 2016). The investigation into behaviour patterns of NPS pollutant clouds within water bodies is uncommon. Study on the hydrodynamic processes which occur within a water body due to NPS loading, and the rate NPS pollutant concentration patterns distribute in-stream cannot be ignored. The difficulties associated with effective prediction of in-stream flux of NPS pollutants is that requires a simplified and easy to interpret model, which must be able to balance the model complexity with available data.

Theoretical Framework

Mathematical models are generally based on the fundamentals of conservation of mass which combined with Fick's law of diffusion represents the spatial and temporal effects of advection and dispersion of contaminants in water bodies. Research over time identified limitations in the foremost Advection-Dispersion Equation (ADE) leading to the development of other models like the Cells in Series (CIS) and Aggregated Dead Zone (ADZ) models. The practical application of ADE is flawed due to its inability to adequately interpret observed tracer profiles where uniform mixing due to turbulence occurs (Lees et al. 2000). Accuracy in simulating tracer profiles which are dependent on the dispersion coefficient within the stream has also been observed as a flaw of the ADE model (Bencala and Walters 1983, Lees et al. 2000, Ghosh et al. 2004, 2008, Muthukrishnavellaisamy et al. 2009). The CIS model was considered as an alternative to the ADE which reduces the second-order differential equation of the ADE to a first-order differential equation. However, as the CIS model considers individual cells as thoroughly mixed, the advection component is insufficiently simulated, thus, limiting its use in natural streams (Ghosh et al. 2008, Kumarasamy 2015). The ADZ model recognizes storage zones in stream beds and banks, which is considered a significant factor for dispersion within water bodies. It decouples advection and dispersion which allows pure time delay for advection to occur. Thus, adequately describes observed concentration profiles in natural streams. However, parameter estimation and determination of the model orders are the primary challenges with ADZ (Lees et al. 2000; Ghosh et al. 2008). Other models which have been considered as suitable alternatives to ADE model, include the Transient storage model (TS) (Bencala and Walters 1983) modeled in line with the ADZ model, and the Hybrid Cells in Series model (HCIS) (Ghosh et al. 2004, 2008).

Transient Storage (TS) Model
The transient storage (TS) model is a modification of the aggregated dead zone (ADZ) model and adds the process of transient storage to ADZ, which accounts for the elevated tails and skewness in its C-t profiles. It considers shear flow in uniform channels to simulate dispersion within a stream. TS model divides flows in rivers into two zones comprising the stream channel where transport mechanisms of advection and dispersion occur, and a transient storage

zone where portions of solutes are trapped and isolated from the stream channel in underflow channels. It is conceptualized on the basis that as the pulse of solute moves along a stream, the concentration of the solute in the stream channel is attenuated while some solute mass remains within the storage zones. As the pulse passes through the stream channel, the retained solute in the storage zone is released back into the stream resulting in a gradual tailing of the C-t profile. The governing equations of TS model describing a one-dimensional solute transport under steady and uniform flow conditions are:

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E \frac{\partial^2 C}{\partial x^2} + \alpha (C_s - C) \tag{1}$$

$$\frac{\partial C_s}{\partial t} = \alpha \frac{A}{A_s} (C_s - C) \tag{2}$$

Where C and C_s (mgl^{-1}) are the solute concentrations in the stream channel and storage zone respectively, and A and A_s (m^2) represent the cross-sectional area of the stream channel and storage zone. The average flow velocity of the reach is denoted by u (ms^{-1}), E (m^{2}s^{-1}) is the longitudinal dispersion coefficient while α (s^{-1}) denotes the stream storage exchange coefficient, t (s) represents time while × (m) denotes distance. The coupling term α (c_s–c) in Eqs (1) and (2) appear simple. However, the numerical solutions of both equations require as many as three parameters for calibration. Estimating these parameters is difficult and complicated (Lee et al. 2000). Progressive work on TS model has seen the inclusion of several processes including lateral inflow and first-order decay components.

Hybrid Cells in Series (HCIS) Model
The HCIS model is a conceptual model whose process is based on the physiognomies of the mixing cells concept. The model describes pure advection through time delay within each cell with dispersion occurring when each cell is assumed as thoroughly mixed. It is a three-parameter model, which represents the Gaussian distribution of continuous-time. The HCIS considers a stream network as a series of hybrid units and each unit consists of three cells namely, a plug flow cell characterized by pure advection indicative of no change in solute concentration, and two distinct mixing cells where advection and dispersion processes occur. Each cell has independent residence times in which fluids flowing through each cell is replaced. The residence time in the plug flow cell is denoted as α equal to V_0/Q, while the residence time in the first and second mixing cells are denoted as T_1 and T_2, equated to V_1/Q and V_2/Q respectively; where Q is flow rate, and V_0, V_1, and V_2 represent the volume of the plug flow, first and second mixing cells. These residence time parameters describe the first arrival time of pollutant concentration front, peak concentration, spread (dispersion) and skewness. The size of the hybrid unit Δx must satisfy the Peclet number condition of Pe= $\Delta x u$ /D_L ≥ 4; when u is mean flow velocity and D_L is longitudinal dispersion coefficient to correctly simulate advection and dispersion processes of pollutant transport (Ghosh et al. 2004; 2008).

The parameters α, T_1, and T_2 can be estimated using the least square optimization method which is considered preferable to the method of moments and method of partial moment, the time to peak and peak concentration (Ghosh et al. 2008). Though, HCIS was conceptualized initially to simulate conservative pollutants in streams and rivers. Kumarasamy et al. (2011, 2013) implemented the inclusion of pollutant sorption and decay processes to the model. Kumarasamy (2015) also simulated DO concentration in streams by adding up De-oxygenation and Re-aeration component to HCIS model, while Olowe and Kumarasamy (2017) demonstrated its suitability for simulating ammonia in rivers by incorporating the first-order kinetic equation for ammonia nutrients. The flexibility and adaptability of the HCIS model form the basis for its use in developing a new model component for simulating in-stream NPS pollution. This paper presents the process of deriving a model based on the HCIS concept for simulation of NPS pollutants in streams. The new model will be verified using synthetic data and field data retrieved from existing literature.

Method

Derivation of Model Equations

As with most water quality models, differential equations are derived using the fundamental concept of conservation of mass. In deriving the governing equations, a mass balance is carried out on a stream segment considering a stream of control volume ΔV, length Δx, and cross-sectional area A, having a mass flow entering at the upstream end of the channel and a uniformly distributed lateral surface inflow entering along the channel, as expressed in O'Conner (1976). Neglecting longitudinal dispersion, and assuming conservative pollutant, the mass balance at Δt yields

$$\Delta VC = QC\Delta t + C_L\Delta Q_L\Delta t - \left(C + \frac{\partial C}{\partial x}\Delta x\right)\left(Q + \frac{\partial Q}{\partial x}\Delta x\right)\Delta t \quad (3)$$

Take $V = A\Delta x$ and neglecting all higher derivatives, Eq. (3) becomes

$$\frac{\partial}{\partial t}(AC) = -C\frac{\partial Q}{\partial x} - Q\frac{\partial C}{\partial x} + C_L\frac{\partial Q_L}{\partial x} \quad (4)$$

Simplifying Eq. (4) and applying St Venants continuity Eq. (5),

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} - q_L = 0 \quad (5)$$

Yields Eq. (6)

$$\frac{\partial C(x,t)}{\partial t} = -u\frac{\partial C(x,t)}{\partial x} + \frac{q_L}{A}(C_L - C) \quad (6)$$

Eq. (6) is a first-order differential equation consistent with Bencala and Walter (1983) for conservative pollutants in water bodies, excluding dispersion and transient storage component. It is also valid for plug flow component of Hybrid Cells in Series Model (HCIS) (Ghosh et al. 2004). It, therefore, forms the governing equation for HCIS-NPS model, where, $C(x, t)$ is pollutant concentration in the water body (mgl⁻¹), u is flow velocity (ms⁻¹), t is time interval of pollutant displacement (s), x is distance from source (m), q_L is lateral inflow (m³s⁻¹m⁻¹), C_L is pollutant concentration in lateral inflow (mgl⁻¹), and A is the cross-sectional area of the water channel (m²). Incorporating St Venants equation of continuity for unsteady flow in the equation enhances its capability to simulate pollutant transport process under both steady and unsteady flow conditions.

Pollutant concentration in plug flow component of the hybrid unit with non-point source pollution

Applying the governing equation derived in Eq. (6), consider a conservative pollutant is transported downstream a river, made up of a series of hybrid units consisting of a plug flow cell and two thoroughly mixed cells. Assume uniformly distributed inflow of NPS pollutants into the river reach from its bank as shown in (Fig. 1).

Let q_L/A be denoted as ψ and initial and boundary conditions be $C(x, 0) = 0$; $x > 0$, $C(0, t) = C_R$; $t \geq 0$ and $C(\alpha u, t) = 0$; $0 < t < \alpha$, where the initial boundary concentration of pollutants in each cell C_i changes to C_R within the cell. Eq. (6) becomes the partial differential equation for the plug flow cell. Using Laplace transforms and integration, Eq. (6) when $C(0, t) = C_R$; $t \geq 0$ at $x = 0$, $C = C_R + C_L$ and, $C^* = C_R/S + C_L/S$, yields
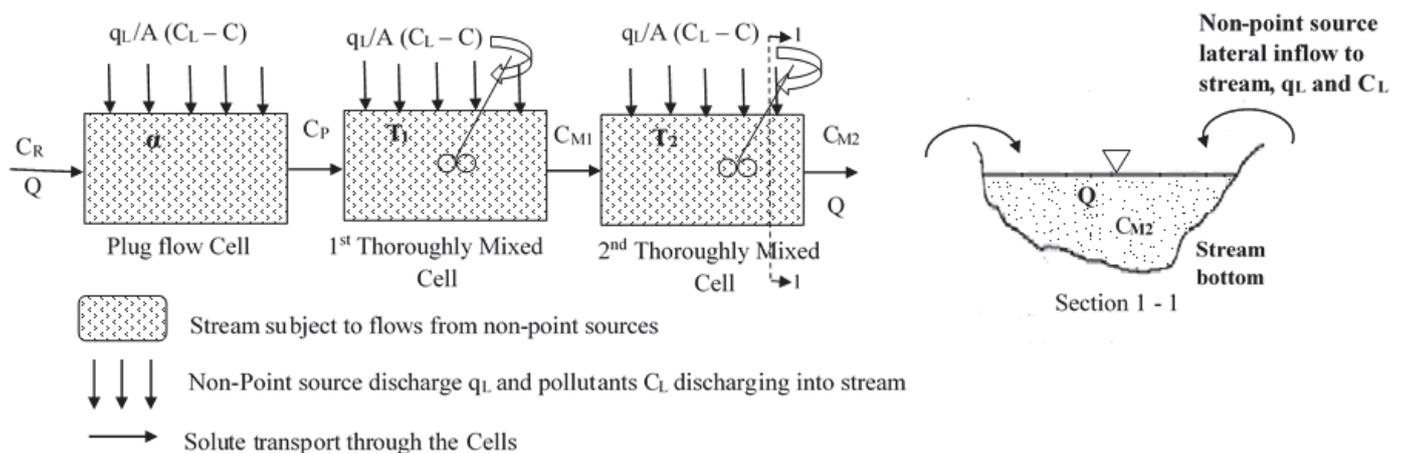

Fig. 1. HCIS Unit inclusive of Uniformly Distributed Lateral flow

$$C_{pf}\left(\alpha u,t\right) = C_R U\left(t-\alpha\right)\exp^{-\psi\alpha} + C_L U\left(t-\alpha\right)\exp^{-\psi\alpha} - \\ -\psi C_L U\left(t-\alpha\right)\exp^{-\psi t} + \psi C_L \exp^{-\psi t} \tag{7}$$

where, C_{pf} is the pollutant concentration at the end of the plug flow cell with NPS contribution. Valid for $t \geq \alpha$, where U $(t-\alpha)$ is the step function.

First mixing cell

Effluent from the plug flow becomes in-stream influent for the first mixing cell. NPS pollutants are also introduced into the system. The mixing cell has a fill time of T_1 as defined earlier. The mass balance for the first mixing cell becomes

$$V_1 \Delta C_{MC1} = C_{pf} Q \Delta t - C_{MC1} Q \Delta t + \frac{q_L}{A}\left(C_L - C_{MC1}\right)V_1 \Delta t \tag{8}$$

where the term on the left, represents the change in pollutant concentration in the cell. The first term on the right is the effluent mass leaving the plug flow into the cell. The second term represents the effluent moving through the mixing cell, while the third term represents the uniformly distributed lateral inflow. Substituting Eq. (7) into (8) and simplifying in differentials yields

$$\frac{dC_{MC1}}{dt} = \left\{ \begin{bmatrix} \frac{C_R U(t-\alpha)\exp^{-\psi\alpha}}{T_1} + \frac{C_L U(t-\alpha)\exp^{-\psi\alpha}}{T_1} - \frac{\psi C_L U(t-\alpha)\exp^{-\psi t}}{T_1} + \frac{\psi C_L \exp^{-\psi t}}{T_1} \\ + \psi C_L - \left[\frac{1+\psi T_1}{T_1}\right] C_{MC1} \end{bmatrix} \right\} \tag{9}$$

$$C_{MC1} = \left\{ \begin{bmatrix} \frac{C_R U(t-\alpha)\exp^{-\psi\alpha}}{1+\psi T_1}\{\Re\} + \frac{C_L U(t-\alpha)\exp^{-\psi\alpha}}{1+\psi T_1}\{\Re\} + \frac{\psi C_L T_1}{1+\psi T_1}\{\Re\} - \psi C_L U(t-\alpha)\{\Im\} \\ + \psi C_L \{\Im\} \end{bmatrix} \right\} \tag{10}$$

where:

$$\Re = \left[1 - \exp^{-\left[\frac{1+\psi T_1}{T_1}\right](t-a)}\right], \qquad \Im = \left[\exp^{-\psi t} - \exp^{-\psi\alpha}\exp^{-\left[\frac{1+\psi T_1}{T_1}\right](t-a)}\right]$$

The solution of Eq. (9) yields the pollutant concentration at the end of the first mixing cell Eq. (10). C_{MC1} is the pollutant concentration from both point and NPS at the end of the first mixing cell.

Second Mixing Cell

Effluent from the first mixing cell becomes influent to the second mixing cell with the inclusion of a uniformly distributed lateral inflow. The residence time within this cell is T_2. Hence, performing mass balance for the second mixing cell at time intervals of t to t + Δt, where all terms of change in pollutant concentration within the cell, effluent mass entering and moving through the second mixing cell and lateral inflow are all accounted for, with step input of C_R, reduces to

$$C_{MC2} = K_{HCIS-NPS} = \left\{ \begin{matrix} \frac{C_R \exp^{-\psi\alpha} U(t-\alpha)}{1+\psi T_1}\{\varepsilon\} + \frac{C_L \exp^{-\psi\alpha} U(t-\alpha)}{1+\psi T_1}\{\varepsilon\} - \psi C_L U(t-\alpha)\{\chi-\varpi\} \\ + \frac{\psi C_L T_1}{1+\psi T_1}\{\varepsilon\} + \psi C_L\{\chi-\xi\} + \psi C_L T_2\{\Gamma\} \end{matrix} \right\} \tag{11}$$

Where:

$$\varepsilon = \left[\frac{1 - \exp^{-\left[\frac{1+\psi T_1}{T_1}\right](t-a)}}{1+\psi T_2} - \frac{T_1\left(\exp^{-\left[\frac{1+\psi T_1}{T_1}\right](t-a)} - \exp^{-\left[\frac{1+\psi T_2}{T_2}\right](t-a)}\right)}{T_1 - T_2} \right]$$

$$\chi = \left[\exp^{-\psi t} - \exp^{-\psi\alpha}\exp^{-\left[\frac{1+\psi T_2}{T_2}\right](t-a)} \right]$$

$$\varpi = \left[\frac{T_1 \exp^{-\psi\alpha}\left(\exp^{-\left[\frac{1+\psi T_1}{T_1}\right](t-a)} + \exp^{-\left[\frac{1+\psi T_2}{T_2}\right](t-a)}\right)}{T_1 - T_2} \right]$$

$$\xi = \left[\frac{T_1 \exp^{-\psi\alpha}\left(\exp^{-\left[\frac{1+\psi T_1}{T_1}\right](t-a)} - \exp^{-\left[\frac{1+\psi T_2}{T_2}\right](t-a)}\right)}{T_1 - T_2} \right]$$

$$\Gamma = \left[\frac{1 - \exp^{-\left[\frac{1+\psi T_2}{T_2}\right](t-a)}}{1+\psi T_2} \right]$$

Eq. (11) is the pollutant concentration at the end of the second mixing cell. It represents the step response of pollutant concentration in the first hybrid unit for a unit step input valid for $t \geq \alpha$. When U $(t-\alpha) = 0$ for $t < \alpha$ and U $(t-\alpha) = 1$ for $t \geq \alpha$. The step response function is designated as $K_{HCIS-NPS}$. Differentiating Eq. (11) with respect to 't' produces the impulse response function of the hybrid unit. Pollutant concentration at the end of 'n^{th}' hybrid unit, for 'n' number of hybrid units in a river reach, is estimated using method of convolution.

Results and Discussions

Model Testing with Synthetic Data

The efficacy of a model can be determined using synthetic data in the absence of relevant and appropriate data. Synthetic data is used in validating the HCIS-NPS model to verify its capability in accounting for NPS loading and in-stream simulations. The model was tested under five scenarios to demonstrate its response to NPS loading. Data sets were generated based on real but random river geometries and used to calibrate the size of each hybrid unit and estimate the resident time α, T_1 and T_2 in each cell of the hybrid. Values for lateral flow (q_L) and pollutant concentrations (C_L) are assumed. In-stream background concentration and point source influent (C_R) is set at 1.0 mg/l. The parameters used in validating the model are given in Table 1.

The simulated concentration profiles at the end of the 1st and 5th hybrid units for different NPS inputs is presented in (Fig. 2). In general, the C-t profiles all demonstrated a drop in peak concentrations as the pollutant moved from the near field to the far-field, producing a long tail in the falling limb. The C-t profiles for scenario 1, is consistent with profiles produced for natural in-stream flows from point sources. In this situation, instream conditions are constant and exclude lateral inflow. Scenario 2 simulated with the inclusion of pollutant-free lateral inflow, shows immediate instream dilution with a reduction in background pollutant concentration. In scenario

4, lateral inflow is further increased but with the addition of minimal pollutant concentration. The profile first experiences a spike in pollutant concentration due to C_L after which dilution occurs. Increase in q_L raises instream flow rate, resulting in dilution within the water body. Attenuation in this instant is not associated with decay or reactions taking place in the water body considering the pollutant is conservative. In this instance, the concentration profile of pollutant downstream the river is not solely dependent on its characteristics, but on timescales and in-stream flows occurring in the waterbody. In Scenario 5, C_L is higher than C_R with reduced q_L. Thus, instream concentration is raised, exceeding boundary concentrations. The C-t curves produced by the model simulation demonstrates that the inclusion of lateral flow in the river results to variations in pollutant concentration from the near field to the far-field of the river. The response of the model to different lateral flow rates q_L alongside pollutant concentration of the flow C_L is consistent with expected patterns.

Validation with Field Data

The performance of the model is tested using the well-documented field data for the Snake River, Colorado, USA. (Fig. 3) (Bencala et al. 1990). The data as shown in Table 2 includes actual distances downstream of the injection point, stream cross-sectional area, dispersion coefficient D_L, lateral inflow q_L and lateral pollutant concentrations C_L. The proposed HCIS-NPS model does not comprise a transient storage component. Therefore, data for transient storage in Bencala et al. (1990) is excluded. The C-t profiles generated using HCIS-NPS is compared with the observed data from Bencala et al. (1990).

In the field experiment as conducted by McKnight and Bencala (1989) 10.49 mol/l of Lithium chloride, a conservative salt, is injected continuously over a 6-hour period into the Snake River at a rate of 86.6mL/min starting at 09hrs. The discharge rate at inception is 0.224m³/s, with a Lithium background concentration of zero as presented in Bencala et al. (1990).

Table 1. HCIS-NPS Model Synthetic Data

Scenarios	Q (m³/s)	U (m/s)	D_L (m²/s)	A (m²)	Δx (m)	α (s)	T_1 (s)	T_2 (s)	C_R (mg/L)	C_L (mg/L)	q_L (m³/s/m)
1	6.67	0.333	16.67	20	250	150	187.8	412.8	1.0	0.0	0.0
2	6.67	0.333	16.67	20	250	150	187.8	412.8	1.0	0.0	0.16
3	6.67	0.333	16.67	20	250	150	187.8	412.8	1.0	0.8	0.16
4	6.67	0.333	16.67	20	250	150	187.8	412.8	1.0	0.8	1.6
5	6.67	0.333	16.67	20	250	150	187.8	412.8	1.0	1.8	0.16
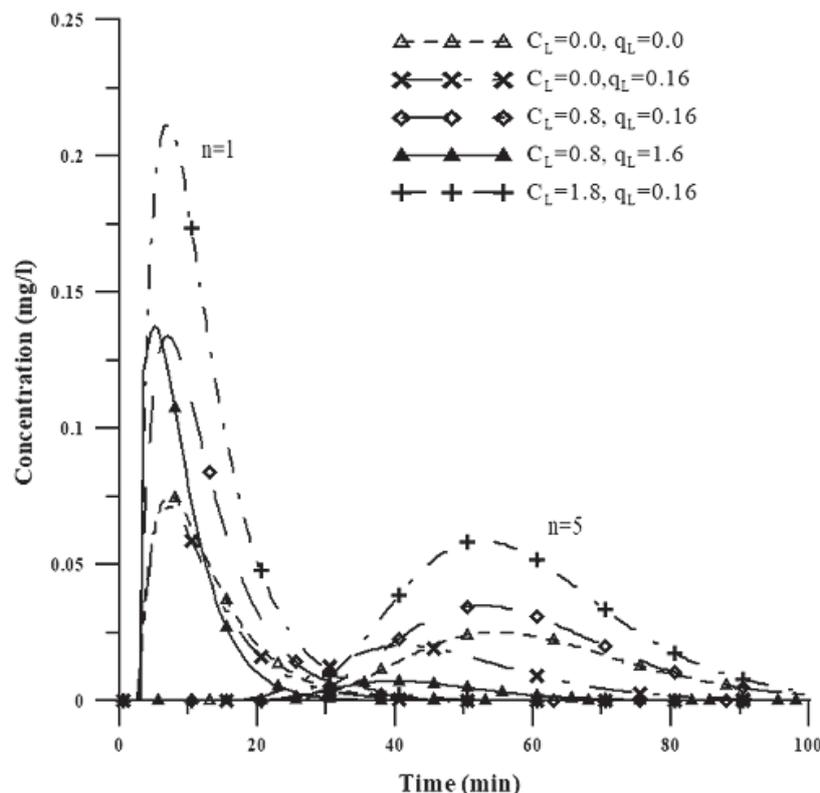
Fig. 2. Unit impulse response of HCIS-NPS model at end of 1st (n=1) and 5th (n=5) Hybrid units when C_L=0, q_L=0; C_L=0, q_L=0.16; C_L=0.8, q_L=0.16; C_L=0.8, q_L=1.6 and C_L=1.8, q_L=0.16

Further downstream after the confluence with Deer creek as shown in (Fig. 3), an increase in discharge rate of 0.81m³/s occurs resulting from inflow from Deer Creek and consecutive distributed inflows. All field procedures and data are detailed in McKnight and Bencala (1989) and Bencala et al. (1990). The HCIS-NPS model simulation is performed at locations closer to the sampling points 628m, 2845m from injection point and, 3192 and 5231m after Deer Creek confluence as shown in (Fig. 3). Each reach length is divided into hybrid process unit sizes Δx, which is determined from the given D_L and computed $U = Q/A$ when the condition of $Pe=\Delta xu/D_L \geq 4$ is satisfied. The resident time parameters α, T_1 and T_2 of the hybrid unit are determined as outlined in Ghosh et al., 2004. All the parameters are estimated and presented in Table 3. Due to variations in the flow rate along the ri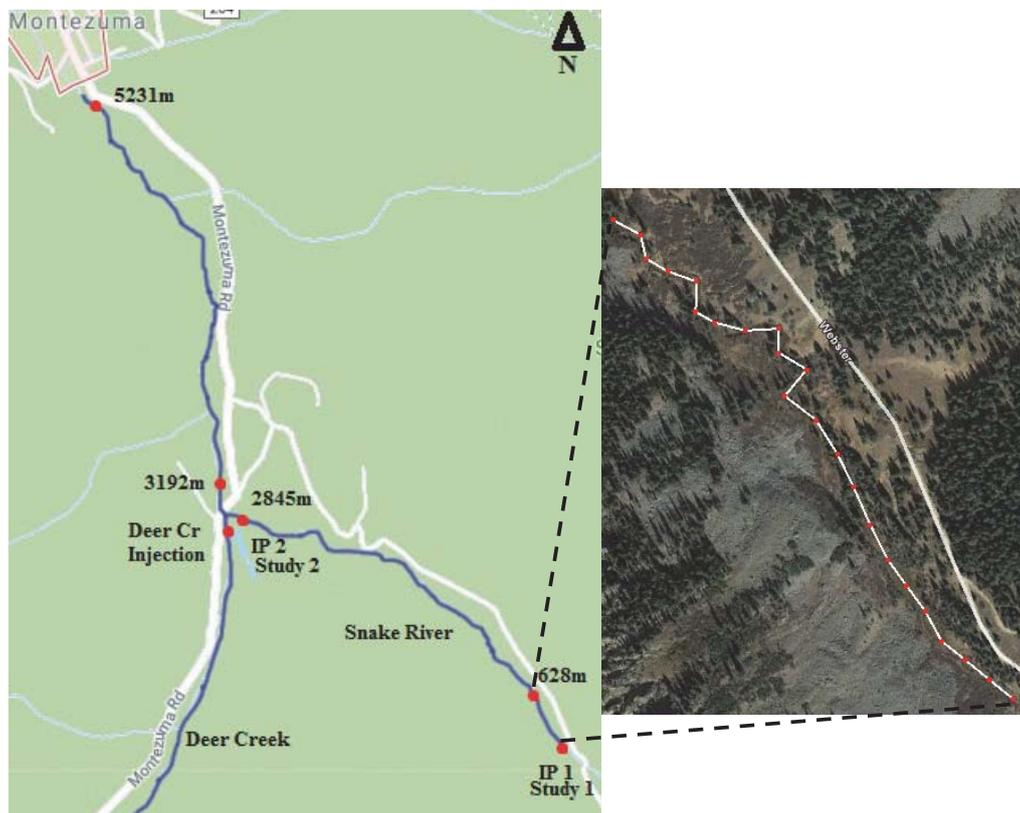ver reaches, the model parameters vary from reach to reach. The flexibility of the HCIS model lies in adopting flow variations through varying model parameters from reach to reach. This is achieved by selecting hybrid unit sizes in each river reach (Table 3).

The simulations in Bencala et al. (1990) were interpreted in square pulses of arrival time zero with a rapid increase in concentration. Figs. 4 and 5 present the C-t curves of the observed data and simulated results from HCIS-NPS model downstream after the injection point and further downstream after the confluence. The simulated results from proposed HCIS-NPS model compare well and are in good agreement with the observed data as shown. Although the observed measurements had some irregular peaks more prominent in the first reach, the simulated and observed concentration curves for 628m match satisfactorily with the leading and trailing

Table 2. Extracted tracer tests data for selected points of Snake River and Deer Creek

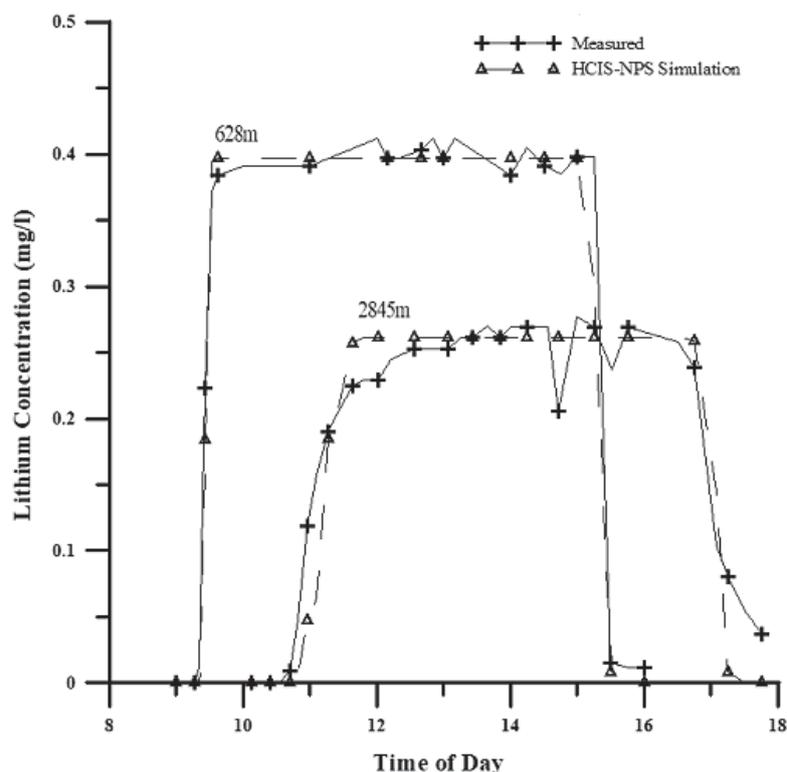| Sampling points (m)	Stream cross-sectional area A (m²)	Computed flow rate U (ms⁻¹)	Dispersion coefficient D_L (m²s⁻¹)	Lateral Inflow q_L x 10⁻³ (m³s⁻¹m⁻¹)	Lateral solute inflow C_L (μM)
Before Confluence					
628	0.61	0.37	0.75	0.062	5
2845	0.70	0.32	0.20	0.028	5
After Confluence					
3192	1.08	0.75	0.20	0.176	4
5231	1.60	0.51	0.20	0.090	4

Source: Bencala et al. (1990)

Fig. 3. Snake River study area map used in McKnight and Bencala (1989) showing injection point, selected sampling sites and delineation of Hybrid units. Source: Google Map

edges of the arrival time produced accurately. At 2845 m the HCIS-NPS model presents a late arrival time which rapidly peaks consistent with the observed data. This lag could be due to the boundary conditions used and a difference in the time and space discretization in the HCIS-NPS model since each sampling site is split into several hybrid units. It could also be attributed to hyporheic exchange occurring within the stream which is not considered in the present model. Downstream after the confluence with Deer Creek, simulated to observed C-t curves for both 3192 m and 5231 compared well with increased and varying discharge rates. However, the falling limb of the simulated curve at 3192m arrived earlier than the observed curve, while at 5231m there was a minimal lag in arrival time. In all cases, however, pollutant concentrations increased sharply to plateau levels at initial arrival to sampling sites, exhibiting characteristic trends. The peak levels of the pollutant decreased in consecutive sampling sites downstream to the injection point. The performance of the observed to simulated data was tested at a confidence level of 95% for all reaches. The coefficient of determination (R^2) is 0.9842 and 0.9382 for 628 m and 2845 m, while for reaches 3192 and 5231, R^2 is 0.8352 and 0.9712. Further, the standard error (SE) for reaches 628 m and 2845 m are 2.279E-2 and 2.697E-2 while 3192 m and 5231 m are 2.321E-2 and 9.35E-3 respectively. The results show a good correlation between the C-t profile of the observed data and the simulated data. The results also indicate the ability of the proposed model to simulate pollutant transport in rivers from non-point sources with variation in flow rate as shown downstream. The output of the proposed HCIS-NPS model was not compared with the simulations of the TS model undertaken in Bencala et al. (1990). The purpose of using the field data in simulating the model was to establish its suitability and capability for use in NPS in-stream simulation.

Table 3. Parameters used for HCIS-NPS simulations of Snake River and Deer Creek

Resident Time			Δt(s)	U(ms^{-1})	D_L(m^{2}s^{-1})	Pe	Δx(m)	No of Hybrid units	Calculated distance from IP (m)	Actual Distance from IP (m)
α(s)	T_1(s)	T_2(s)								
Before Confluence										
27	33.65	0.619	0.5	0.37	0.75	11	22	28	616	628
9.453	11.816	0.214	0.5	0.32	0.20	11	7	316	2828	2845
After Confluence										
1.721	2.151	0.039	0.5	0.75	0.20	11	3	115	3173	3192
3.772	4.652	0.086	0.5	0.51	0.20	11	4	509	5209	5231

Fig. 4. Comparison of C-t profiles for the observed data with results simulated by proposed HCIS-NPS model at 628 m and 2845 m downstream from tracer injection point
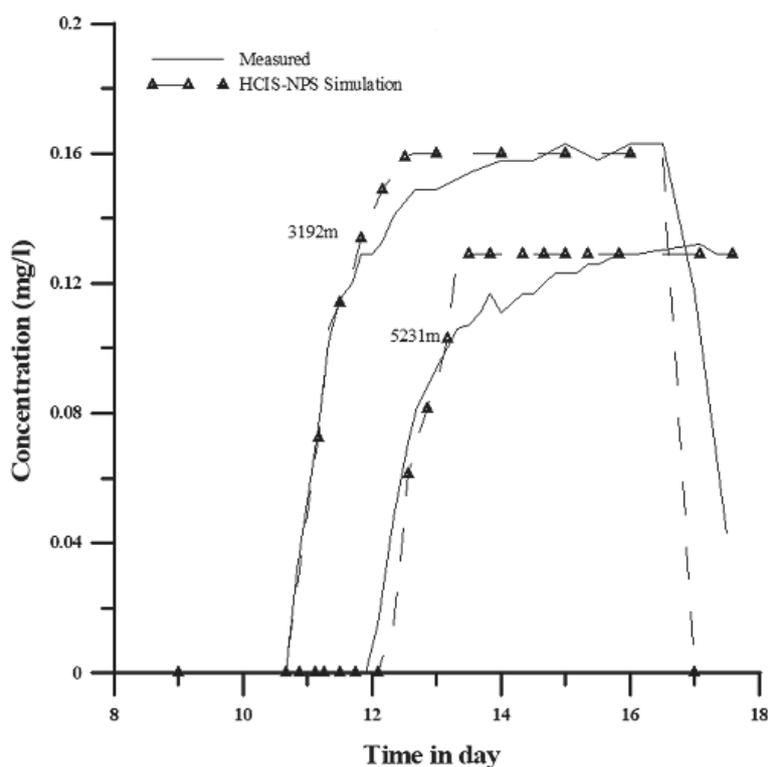
Fig. 5. Comparison of C-t profiles for the observed data with results simulated by proposed HCIS-NPS model at 3192 m and 5231 m from tracer injection point after Deer creek confluence

Conclusion

In this study, an HCIS-NPS model has been proposed for simulating the transport of pollutants in water bodies affected by non-point source pollution. A non-point source component was incorporated to the general HCIS model which has been tested for its flexibility and adaptability for varying water quality processes and is found to overcome the flaws and complexities associated with the fickian based and other mixing cell models. Although the TS model was reviewed, the purpose of the paper is not comparative but rather to validate the performance of the proposed HCIS-NPS model using field data from Bencala et al. (1990). The response of the C-t curves produced by the model for both synthetic data and field data demonstrates its ability to effectively simulate pollutant transport in a natural river inclusive of non-point source pollution. It also demonstrates its ability to simulate in-stream processes with varying discharge rates. It can be concluded that the simplicity of the HCIS-NPS model, regarding its ease of operation, parameter estimation and reduced run-time, makes it suitable, convenient and easy to use. Thus, considering the difficulties associated with other available NPS models, HCIS-NPS model is a useful tool for predicting pollutant transport in water bodies with non-point source pollution. This model would require to be further extended to simulate non-conservation pollutants and Hyporheic exchange.

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