SIMULATION OF MASS TRANSFER IN A RIVER WITH DEAD ZONES USING NETWORK SIMULATION METHOD

by

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In this study, network simulation method is applied to solve a 1-D solute transfer problem governed by transient storage model in a mountain stream including dead zones. In this computational method, for each node of the discretized domain, the terms of governing equation are substituted by the equivalent electrical devices which are connected to each other based on Kirchhoff's current law. Finally, the total electric circuit is solved using an appropriate electrical code to obtain the unknown value at the nodes. Because no analytical solutions for this model have been presented so far, to verify network simulation method, the problem is solved by finite volume method, as well. According to the results, estimations made by network simulation method and finite volume method are in good agreement. Further, network simulation method is easier in implementation, especially in implementation of boundary conditions, and faster than finite volume method in computation. Therefore, in the case of 1-D mass transfer problems with a set of coupled equations, network simulation method is recommended to be used as an efficient alternative to numerical methods.

Key words: *mass transfer, transient storage model, network simulation method, finite volume method, river*

Introduction

Water pollution as the main cause of deaths all over the world is an important worldwide concern. Based on reports, human activities everyday release a large amount of domestic, industrial and agricultural waste into water bodies and continuously influence and change the ecosystem conditions in the world. Regarding the harmful and irrecoverable environmental effects of these pollutions, studies on predicting and controlling these pollutions in the streams are essential [1].

For this purpose, the well-known classical advection-dispersion equation (ADE), which is based on the principle of continuity and Fick's first law, was presented as the first effort for describing mass transfer and energy transfer in physical systems. The general form of this equation can be found in [2, 3]. According to the experimental studies carried out in rivers by several authors, ADE is no longer applicable for natural streams because of their irregular cross-sections [4-7]. Afterward, more accurate models referred to *dead zone* models or

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transient storage (TS) models were developed and calibrated by several researchers using tracer approach in rivers. Such models caused more compatible results, that is the concentration-time distributions with lower picks and longer tails, *e. g.* [5, 8-12].

In these models the hydrologic system has been divided into two interacting parts: the flowing stream channel and the transient storage zones. The effect of exchange with surface transient storage zones including in-channel low velocity areas (so-called dead zones) caused by irregularities in the riverbed (obstructions, vegetation, meander bends and lateral cavities) and as well, the hyporheic zones including the porous media of channel bed and banks, in temporal retention of solute and increasing the reactions, are considered. In this model, the whole dead zones are considered as a completely stirred reactor. To find more about this model and such other models refer to [8, 13].

One of the most useful models for describing the solute transport in rivers which has been solved by many authors using different numerical methods and has been used in this study is developed by Bencala and Walters [14] and Bencala [8] for conservative and reactive solute, respectively. In this model, known as TS model, the physical transfer mechanisms in the main channel include advection, dispersion, exchange due to the transient storage and lateral inflow/outflow. Whereas, based on assumptions made by them, the only physical transport mechanism in the storage zone is solute exchange with the main channel. The chemical reaction of the solute, including the decay and sorption of solute by the streambed sediments, is treated as a first-order reaction in both the main channel and storage zone. The model equations are presented in the following section. To find studies in which TS model has been used to simulate solute transport in natural streams see [7, 9, 14-21].

In this study, the mentioned reactive mass transfer coupled model equations are solved by a powerful, accurate and fast computational approach referred to network simulation method (NSM), an approach that, as claimed by Alhama and Campo [22], was used for the first time in 1942 by Paschkis and Baker to simulate a heat transfer problem. In this method using the equivalent electrical devices, the governing differential equations of the system are electrically simulated. As stated by the past researchers, this novel approach, because of its ability to simulate the non-linear and coupled mechanisms using non-linear electrical devices, is somewhat more capable than the classic electrical analogy [23, 24].

The NSM has been implemented successfully in case of linear and non-linear problems including heat transfer, mass transfer and chemical reactions, charge transfer and force transfer, which some examples can be found in [23, 25-31]. Unlike previous mass transfer simulations which were mostly performed in a bulk low-velocity media such as groundwater and estuaries [25, 28, 30, 32], in this simulation, advection and solute exchange mechanism with dead zones are also considered. Caravaca *et al.*, [33], have claimed that in the case of solving the ODE, NSM reaches the solution much faster than standard simulation algorithms such as fourth order Runge-Kutta algorithm. Based on many studies, NSM is usable for any complex kinetic process without necessity of theoretical approximations and because of its short calculation time, it is suitable for simulating the long term processes which need long times to reach their steady-state. Some examples of these processes are presented in [27, 29, 33].

Since it has not been presented any analytical solution for the studied mathematical model yet, to verify and validate NSM and also, to make a comparison between the efficiency of this method and common numerical methods, we have also solved this problem using finite volume method (FVM), a frequently-used numerical method in CFD, with two manners for discretizing the time derivatives [34].

Materials and methods

Mathematical model

The model equations for 1-D reactive solute transport presented by Bencala [8], as described below, have some additional terms in comparison the classic ADE, accounting for the lateral flow, flow exchange with transient storage zone and reaction with streambed sediments:

$$\frac{\partial c}{\partial t} = -\frac{Q}{A}\frac{\partial c}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial c}{\partial x}\right) + \frac{q_{\text{lat.}}}{A}\left(c_{\text{lat.}} - c\right) + \alpha\left(c_{\text{S}} - c\right) + \tilde{\rho}\lambda\left(c_{\text{Sed}} - K_d c\right) \tag{1}$$

$$\frac{\partial c_{\text{S}}}{\partial t} = \alpha\frac{A}{A_{\text{S}}}\left(c - c_{\text{S}}\right) + \lambda_{\text{S}}\left(\hat{c}_{\text{S}} - c_{\text{S}}\right) \tag{2}$$

$$\frac{\partial c_{\text{Sed}}}{\partial t} = \lambda\left(K_d c - c_{\text{Sed}}\right) \tag{3}$$

Two adjustable parameters of this model are A_{S} and α which, as claimed by Jackman *et al*. [35], show the ultimate storage capacity and the rate of following of main stream concentration by storage concentration, respectively. A more detailed description about TS model, application and limits of this formulation the mountain streams can be found in [5, 8, 11, 15], *etc*.

Solution approach

The computational approach used in this study to obtain the temporal and spatial behavior of considered variables, NSM, involves some electrical circuits analogous to the target system due to their governing equations. To design such equivalent circuits, the differential equations corresponding to the prototype must be discretized spatially over the studied domain. Then, appropriate electrical elements equivalent to each term are connected to each other following the algebraic sign of the term. After implementing the initial and boundary conditions of unknown variables using appropriate sources, the complete electrical network model will be simulated using an electrical-computational code, such as PSpice code. This process is explained more detailed in [36]. PSpice uses Newton-Raphson iterative algorithm to solve this set of non-linear equations and performing the transient analysis [37].

To investigate the veracity and validity of NSM, FVM has been applied to this problem using two implicit schemes for temporally discretizing the model equations. In the application of FVM, after dividing the physical domain into discrete control volumes, the model equation(s) must be integrated over each control volume to reach a set of linear spatially discretized algebraic equations. This system of equations may be solved for each time-step using different algorithms, depending on the case, to obtain the distribution of unknown variables over time and space.

The spatial discretization schemes used in all simulations of this study, are QUICK scheme (3$^{\text{rd}}$-order) and Central scheme (2$^{\text{nd}}$-order) for first-order and second-order spatial derivatives, respectively. The time derivatives in FVM simulation are discretized using Crank-Nicolson (semi-implicit) and fully-implicit schemes. Crank-Nicolson scheme, which is based on central differencing, results in quadratic errors. Whether fully-implicit scheme, which is based on backward differencing, causes linear errors. Both of these schemes are numerically stable and convergent. For a more detailed description about the application of FVM and discretization schemes in simulation of transfer problems, see [38]

Case study

In this study, the transport of solute strontium injected in Uvas Creek, a mountain stream, is simulated by NSM using the mathematical model presented in section *Mathematical model*. Based on related reports, injection of the solute was made at the upstream end of a 640-m reach. The 1-D domain of the studied reach has been demonstrated in fig. 1. As seen, there are five monitoring stations (38, 105, 281, 433, and 619 meters distant from the injection point) and also another station (station T) for estimating the background solute concentration in the stream channel. The solution was injected at a relatively constant rate for three hours. The background concentration of strontium was measured to be 0.13 mg/l. The detailed data of the injection and measurements at each station can be found in [14].

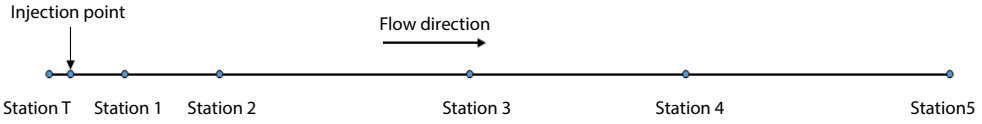

Figure 1. The 1-D scheme of the studying domain, Uvas Creek stream

Simulation parameters estimated by Bencala and Walters [14] and Bencala [8], for solute transfer in Uvas Creek stream, in which they have neglected $q_{\text{lat.}}$ because of its insignificant effect on the final results, are presented. In 1998, Runkel [11] used different values of Q, A_S and $q_{\text{lat.}}$ for the same case to improve the simulation. He set Q as a constant value and attributed its increment to the lateral flow with a solute concentration, $c_{\text{lat.}}$, equal to the background concentration of the main stream. These values, listed in tab. 1, are used in this study.

Table 1. Model parameters [11]

Reach [m]	Q [m^3s^{-1}]	D [m^2s^{-1}]	A [m^2]	A_S [m^2]	α [s^{-1}]	K_d [mlg^{-1}]	$\bar{\rho}$ [gm^{-3}]	λ [s^{-1}]	λ_S [s^{-1}]
0-38	0.0125	0.12	0.30	0.00	0.00	70.0	$0.4 \cdot 10^5$	$0.56 \cdot 10^{-4}$	1.0
38-105	0.0125	0.15	0.42	0.00	0.00	70.0	$0.2 \cdot 10^5$	$0.56 \cdot 10^{-4}$	1.0
105-281	0.0133	0.24	0.36	0.36	$0.30 \cdot 10^{-4}$	70.0	$0.2 \cdot 10^5$	$0.56 \cdot 10^{-4}$	1.0
281-433	0.0136	0.31	0.41	0.41	$0.10 \cdot 10^{-4}$	70.0	$0.2 \cdot 10^5$	$0.56 \cdot 10^{-4}$	1.0
433-619	0.0140	0.40	0.52	1.56	$0.45 \cdot 10^{-4}$	70.0	$0.4 \cdot 10^5$	$0.56 \cdot 10^{-4}$	1.0

c_{inj}=1.73 mgl^{-1}, c_b=$c_{S,b}$= $\hat{c}_s$ = $c_{\text{lat.}}$= 0.13 mgl^{-1}, $c_{\text{Sed,b}}$ = 9.1 μgg^{-1}

Application of NSM for the target problem

To make the electroanalogical model, after discretizing the 1-D domain of problem defining an equally-spaced mesh (Δx), and writing the finite difference spatially-discretized form of TS model eqs. (1)-(3) for ith internal cell (i = 3, 4, …, N-1 and N is the number of cells):

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} + \frac{Q_i}{A_i}\left(\frac{c_{i-2} - 7c_{i-1} + 3c_i + 3c_{i+1}}{8\Delta x}\right) - D_i\left(\frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta x^2}\right) + \\ + \frac{q_{\text{lat.}}}{A}\left(c_i - c_{\text{lat.}}\right) - \alpha\left(c_{S_i} - c_i\right) - \tilde{\rho}\lambda\left(c_{\text{Sed}_i} - K_d c_i\right) = 0 \tag{4}$$

$$\frac{\mathrm{d}c_{S_i}}{\mathrm{d}t} + \alpha\frac{A}{A_S}\left(c_{S_i} - c_i\right) - \lambda_S\left(\hat{c}_S - c_{S_i}\right) = 0 \tag{5}$$

$$\frac{\mathrm{d}c_{\mathrm{Sed}_i}}{\mathrm{d}t} + \lambda\left(c_{\mathrm{Sed_i}} - K_d c_i\right) = 0 \tag{6}$$

Mass fluxes for each process:

$$J_{i,\mathrm{tran.}} = \Delta x \frac{\partial c_i}{\partial t},\ J_{i,\mathrm{adv.}} = \frac{Q}{8A}\left(c_{i-2} - 7c_{i-1} + 3c_i + 3c_{i+1}\right),\ J_{i,\mathrm{disp.,\,in}} = \frac{D}{\Delta x}\left(c_{i+1} - c_i\right)$$
$$J_{i,\mathrm{disp.,\,out}} = \left(\frac{D}{\Delta x}\right)\left(c_i - c_{i-1}\right),\ J_{i,\mathrm{lat.}} = \frac{q_{\mathrm{lat.}}}{A}\Delta x\left(c_i - c_{\mathrm{lat.}}\right),\ J_{i,\mathrm{ex.}} = \alpha\Delta x\left(c_{\mathrm{S}_i} - c_i\right), \tag{7}$$
$$J_{i,\mathrm{react.}} = \tilde{\rho}\lambda\Delta x\left(c_{\mathrm{Sed}_i} - K_d c_i\right)$$

$$J_{\mathrm{S}_i,\mathrm{tran.}} = \Delta x \frac{\mathrm{d}c_{\mathrm{S}_i}}{\mathrm{d}t},\quad J_{\mathrm{S}_i,\mathrm{ex.}} = \frac{\alpha\Delta x A}{A_{\mathrm{S}}}\left(c_{\mathrm{S}_i} - c_i\right),\quad J_{\mathrm{S}_i,\mathrm{react.}} = \lambda_{\mathrm{S}}\Delta x\left(\hat{c}_{\mathrm{S}} - c_{\mathrm{S}_i}\right) \tag{8}$$

$$J_{\mathrm{Sed}_i,\mathrm{tran.}} = \Delta x \frac{\mathrm{d}c_{\mathrm{Sed}_i}}{\mathrm{d}t},\ J_{\mathrm{Sed}_i,\mathrm{ex.}} = \lambda\Delta x\left(c_{\mathrm{Sed_i}} - K_d c_i\right) \tag{9}$$

Since the advection flux in eq. (7) involves three adjacent nodal values (two at upstream c_{i-2}, c_{i-1}, and one at downstream c_{i-1}), in case of nodes 1, 2, and N, which are in the vicinity of domain boundaries, another treatment is needed. Here we have used a linear extrapolation of c-value at the boundaries in order to create an appropriate mirror node for calculations and then the discretized form of the first order spatial derivative of c for nodes 1, 2, and N, has been re-written:

$$J_{1,\mathrm{adv.}} = \frac{Q}{8A}\left(-10c_{\mathrm{A}} + 7c_i + 3c_{i+1}\right) \tag{10}$$

$$J_{2,\mathrm{adv.}} = \frac{Q}{8A}\left(2c_{\mathrm{A}} - 8c_{i-1} + 3c_i + 3c_{i+1}\right) \tag{11}$$

$$J_{\mathrm{N,adv.}} = \text{—}\left(c_{N-2} - 6c_{N-1} - 3c_N + 8c_{\mathrm{B}}\right) \tag{12}$$

where c_A and c_B are the concentration values at upstream and downstream boundaries, respectively.

In order to select an appropriate electrical device equivalent to each mass flux, regarding the current equation of capacitor $I_C = C(\mathrm{d}V/\mathrm{d}t)$ and Ohm law for a resistor $I_R = \Delta V/R$, concentrations (c, c_{S}, and c_{Sed}) and mass fluxes, J, are considered equivalent to the voltage, V, and electrical current, I, respectively. Based on this analogy ($I \equiv J$, $V \equiv c$), transient terms and dispersive terms can be simulated by capacitors of capacitance $C = \Delta x$ and two equal resistors of value $R = D/\Delta x$, respectively. Advective and the other non-linear multi-variable terms may be represented using voltage-controlled current sources, G, with programmable values. As an example, to simulate the advection term of the ith cell using the dependent source G_{i1}, the input voltages including V_{i-2}, V_{i-1}, V_i, and V_{i+1} equivalent to the corresponding concentrations, are detected and processed to produce the output current $I_{Gi,1} = J_{i,\mathrm{adv.}}$.

Since three differential equations are considered in this model, three separate equivalent circuits are designed for which the Kirchhof's current laws based on eqs. (4)-(9):

$$J_{i,\mathrm{tran.}} + J_{i,\mathrm{adv.}} + J_{i,\mathrm{disp.,\,in}} - J_{i,\mathrm{disp.,\,out}} + J_{i,\mathrm{lat.}} - J_{i,\mathrm{ex}} - J_{i,\mathrm{react.}} = 0 \tag{13}$$

$$J_{S_i,\text{tran.}} + J_{S_i,\text{ex.}} - J_{S_i,\text{react.}} = 0 \tag{14}$$

$$J_{\text{Sed}_i,\text{tran.}} + J_{\text{Sed}_i,\text{ex.}} = 0 \tag{15}$$

The elementary network model for each equivalent circuit configured based on eqs. (13)-(15), is shown in fig. 2. The upstream boundary condition for studying reach includes a steady injection of solute for three hours, which is a Dirichlet type boundary condition and it can be implemented by using a piece-wise linear (PWL) voltage source installed at upstream boundary node. The downstream boundary is assumed as a Neumann type zero-gradient boundary. Considering this condition and using a 2nd-order backward scheme, c-value at the downstream boundary, c_B, has been calculated and it can be simulated by a voltage-controlled voltage source, E, connected to the downstream boundary node:

$$c_B = \frac{29}{24}c_N - \frac{6}{24}c_{N-1} + \frac{1}{24}c_{N-2} \tag{16}$$

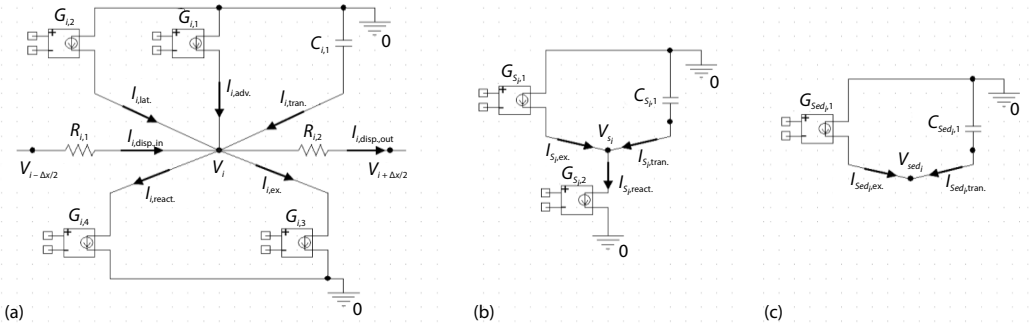

Figure 2. Network model of a spatial element for solute concentration; (a) in the stream, c, (b) in the storage zone, c_S, and (c) on the streambed sediments, c_{Sed}

To obtain the solution, which is the voltage values at each spatial node equivalent to the corresponding concentration values, the designed electrical network is simulated by a PSpice standard circuit analysis code. For transient analysis, PSpice makes an automatically and continuously adjusted time-step to reach convergence at an efficient time-step. Since for a big number of computational nodes, providing the PSpice code in manual manner is time-consuming and capable of errors, here we have used a higher level programming language, Borland C++ Builder 6.0, to produce this code easily through designing an interface form to enter the value of model parameters.

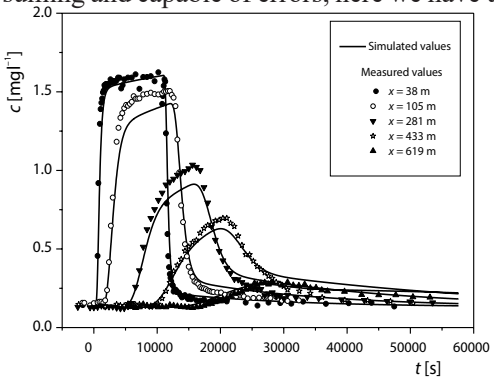

Figure 3. Observed and simulated strontium concentration using NSM for five locations

Using BTQS (Backward-Time, QUICK-Space) and CTQS (Central-Time, QUICK-Space) discretizaion schemes, the FVM computational code for each one, is developed in MATLAB R2015a.

Results and discussion

In this study, a uniform computational space-step of 1.00 meter has been used. To reduce the errors due to the zero-gradient assumption at the downstream boundary, as suggested

by Runkel [11], the last study reach extended an additional 50 meters downstream. After specifying the appropriate boundary condition for each injection case, simulation is performed for a total duration of 16 hours. The time-step is set by PSpice; however, the maximum computational time-step for transient simulation is adjustable. The results of simulation by NSM using parameters of tab. 1 along with the observed values presented in [39], are shown in figs. 3-5.

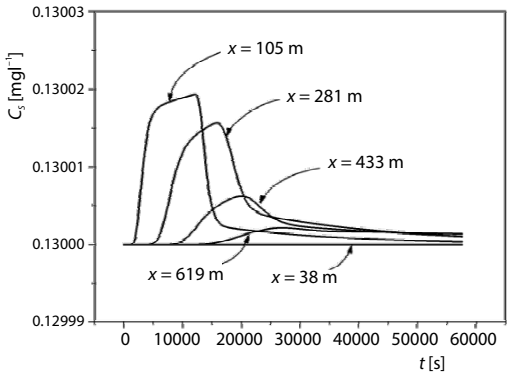

Figure 4. Simulated strontium concentration in storage zone at five stations using NSM

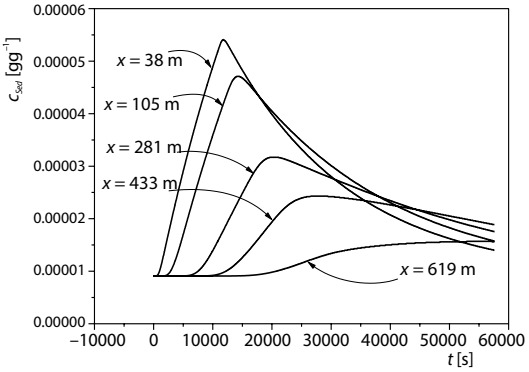

Figure 5. Simulated strontium mass absorbed on bed sediments at five stations using NSM

As mentioned before, FVM has been used to verify and validate the performance of our equivalent electrical model. For this purpose, the results of simulating in-stream solute transfer by FVM, using different discretization schemes (BTQS and CTQS) and different computation time-steps including Δt = 20 s, 25 s, and 50 s, have been compared to the results of simulation by NSM. At first, regarding the previous studies, it has been assumed that NSM is more accurate than the other numerical methods with the same space-step and based on this assumption, the average relative error percentages of FVM simulations for n cross-sections have been calculated:

$$\text{Error}[\%] = \left[\frac{1}{n} \sum_{i=1}^{n} \left(\frac{\left| \text{Integral of } NSM \text{ graph} - \text{Integral of } FVM \text{ graph} \right|}{\text{Integral of } NSM \text{ graph}} \right)_i \right] \cdot 100\% \tag{17}$$

The results of simulation with FVM have been shown in fig. 6 for time-step equal to 50 seconds. The computational errors for simulation of strontium transfer by FVM for different computation time-steps have been presented in tab. 2.

Table 2. Average relative error of simulation strontium concentration by NSM

Method	FVM-BTQS			FVM-CTQS		
Δt [s]	50	25	20	50	25	20
Error [%]	0.28	0.27	0.26	0.32	0.28	0.27

These results indicate that the difference between the simulation results of NSM and FVM is less than 0.3%. In ad-

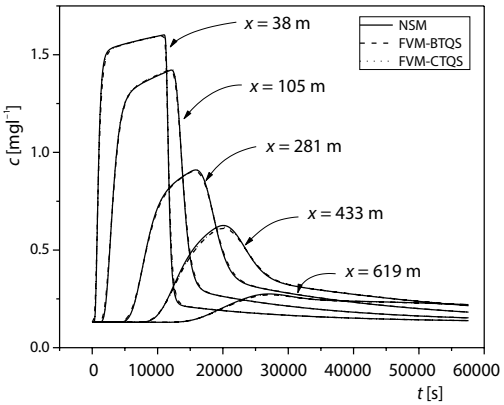

Figure 6. Simulated strontium concentration in the main channel at five stations using NSM and FVM (Δt = 50 s)

dition, considering the trend of changes in errors by changing in time-steps, it can be seen that by reducing the time-steps the differences of results between NSM and FVM is reducing. Therefore, it can be deduced that the first assumption about the accuracy of using methods is valid. As seen, using CTQS scheme, because of its 2nd-order accuracy, the computational error has reduced faster by decreasing the time-steps. The computation times needed for simulating the strontium transfer by NSM and FVM have been listed in tab. 3. As seen, NSM is much faster than the others. It is because of the iterative built-in algorithms employed by PSpice which update the time-step continuously and result in a faster convergence in transient simulations.

Table 3. Computation time for simulation of strontium transfer

Method	NSM	FVM-BTQS			FVM-CTQS		
Δt [s]	–	25	20	10	25	20	10
Time [s]	18.50	214.68	278.82	552.92	231.93	301.56	643.24

* Adjusted by PSpice

Conclusions

Nowadays, because of the increasing environmental crises, monitoring the water quality in rivers, exposed to the pollutants caused by human activities is of high importance. Regarding this necessity, several mathematical models, describing the transfer of mass in aquatic environments, have been developed. Between these models, those ones which are based on the classical ADE, have been more popular. Solving such equations, for which in most of the cases the analytical solution does not exist, needs numerical methods –methods which usually deal with complexity and are time-consuming.

In this study, we have applied NSM – a powerful and efficient computational method for systems governed by differential equations based on the electric circuit conceptsv – to solve TS model, which according to the previous studies, simulates desirably the transport of mass in natural streams. The model has been solved by NSM for a reactive element injected to a mountain river and the results of this simulation, including the concentration in different times and distances, have been compared with the results obtained from FVM – a widely used numerical method- applied to the same case.

The results of simulations illustrated a desirable agreement between NSM and FVM. Furthermore, it is realized that NSM needs far less computation time compared to FVM and provides more accurate estimations of dependent variables. In addition, since in implementation of NSM only the spatial discretization of the model equations is required, its application is easier than the other numerical methods which need both spatial and temporal discretization in their application process. The other advantage of this method is its flexibility in simulation of boundary conditions. Using PSpice as a powerful electronic circuit simulator, has increased the efficiency and performance of this method.

Therefore, it is highly recommended to use NSM in CFD, where the system's governing equations are differential equations, as an appropriate substitute for numerical methods in 1-D simulations for simulating the fluid-flow and solute transfer, providing benchmarks for verifying other computational methods and performing the comparative studies.

Furthermore, since in NSM the designed equivalent electrical circuit is also physically analogous with the prototype, it can be used as a predicting and monitoring tool instead of using

the physical hydraulic models – which are troublesome – in order to perform water quality studies with less time, low expense and high accuracy. Therefore, in critical conditions, including a sudden spill of a high-hazardous contaminant in a specified point of the river or increasing the concentration of a chemical element to its maximum level, the monitoring and controlling measures at different parts of the river can be carried out with an acceptable accuracy and speed to improve the water quality.

Nomenclature

A – cross-sectional flow area, [m^2]
c – solute concentration, [kgm^{-3}]
C – charge capasitance, [Farad]
c_{Sed} – concentration on streambed sediment, [$kgkg^{-1}$]
$\hat{c}$ – equilibrium solute concentration, [kgm^{-3}]
D – dispersion coefficient, [m^2s^{-1}]
I – electric current, [A]
J – mass flux, [$kgm^{-2}s^{-1}$]
K_d – distribution coefficient, [m^3kg^{-1}]
n – number of time-steps, [–]
N – number of space-steps, [–]
Q – volumetric flow rate, [m^3s^{-1}]
q – volumetric inflow rate per length, [m^2s^{-1}]
R – electrical resistance, [Ohm]
t – time, [s]
V – electric potential (voltage), [V]
x – distance, [m]

Greek symbols

α – stream-storage exchange coefficient, [s^{-1}]
Δ – changes in variables
λ – first-order rate coefficient in the stream, [s^{-1}]
$\tilde{\rho}$ – mass of accessible sediment per volume of stream water, [kgm^{-3}]

Subscriptions

adv. – advection
b – background
disp. – dispersion
ex. – exchange
i – space-step counter
in – input
inj – injection
lat. – lateral flow
out – output
react. – chemical reacion
S – storage zone
Sed – streambed sediments
tran. – transient

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