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Numerical Computation of a Water-Quality Model with Advection-Diffusion-Reaction Equation Using an Upwind Implicit Scheme

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Abstract In this research, numerical water-quality model calculations are proposed within a uniform flow stream. The governing equation, which is an equation of advection-diffusion-reaction, is approximated by using a technique of finite differences. The upwind-implicit scheme is used at all times on an uniform flow stream to approximate the pollutant concentration at each point. The accuracy of the proposed computing technique is compared with the analytical, and the examples show approximate solutions.

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1. Introduction

Mathematical simulation is an important method of detecting the assumption of water quality in consideration of location. The methodology of numerical solution is a finite differential approach that can be easily extended to mathematical simulation flow and modelling of transport. Many people use the numerical scheme to approximate the direction of advection-diffusion-reaction equation using the method of finite difference [1–6]. The numerical techniques for solving the uniform flow of stream water quality model, especially the one-dimensional-advection diffusion reaction equation, are presented in [7–11]. In [12] presented the water quality model in a non-uniform flow of stream for one-dimensional hydrodynamic advection-diffusion-reaction equations by using the fully implicit schemes are propose. In [13] developed a new scheme that guaranteed the positivity of the solutions for a one advection-diffusion-reaction equation in one spatial dimension. In [14]

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presented a numerical simulation of a one-dimensional advection-diffusion-reaction equation with boundary condition functions by using the Saulyev finite difference technique. The numerical result was dependable. In the recent year, [15] propose a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes.

The computational methodology suggested allows use of an unconditionally stable system. The numerical experiments give a rational approximation of the calculated effects. In this work, the finite difference technique for approximating the concentration of pollutants on a uniform flow stream using an implicit upwind scheme and modified Siemieniuch-Gladwell scheme is used to measure the concentration of pollutants on a uniform flow stream at all times at each point.

2. The Governing Equation

A one-dimensional water quality model is described the mass transport and diffusion processes. It can be modeled in the advection-diffusion-reaction equations (ADREs).

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}=D\frac{\partial^2 c}{\partial x^2}-Kc, \qquad 0<x<L\ ,\ 0<t\leq T. \tag{2.1}$$

where $c\left(x,t\right)$ is the pollutant concentration $\left(kg/m^3\right)$ of water at the displacement x (m) and time t (s) for all $(x,t)\in(0,L)\times(0,T)$, $u\left(x,t\right)$ is the velocity in x direction (m/s), D is the diffusion coefficient $\left(m^2/s\right)$ and K is the mass decaying rate $\left(s^{-1}\right)$ with the potential pollutant concentration as the initial condition,

$$c\left(x,0\right)=f\left(x\right), \qquad 0\leq x\leq L, \tag{2.2}$$

and the released pollutant concentration on the left boundary and the right boundary

$$(0,t)=g\left(t\right), \qquad 0<t\leq T, \tag{2.3}$$

$$(L,t)=h\left(t\right), \qquad 0<t\leq T, \tag{2.4}$$

the initial condition and the boundary conditions are illustrated in Fig. 1.

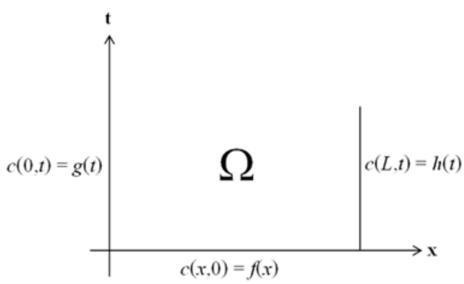

Figure 1. The initial condition and boundary conditions.

3. Numerical Techniques

We consider both implicit and explicit methods to approximate the solution of the advection-diffusion-reaction equations (ADREs).

3.1. A Third-Order Finite Difference Schemes

The solution domain of the problem is covered by a mesh of grid point $x\,(x_i, t_n)$ by $x_i = i\Delta x$, $i = 0, 1, 2, ..., M$, and $t_n = n\Delta t$, $n = 0, 1, 2, ..., N$, where x_i and t_n are parallel to the space and time coordinate axes. We can approximate $c\,(x_i, t_n)$ by c_i^n, value of the difference approximation of $c(x,t)$. The constant spatial and time increment grid-spacing are $\Delta x = L/M$ and $\Delta t = T/N$. From [16], we get the following discretization, the time derivative $t = n\Delta t$ by using forward-difference,

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{3.1}$$

to approximate the advective term in the advection-diffusion-reaction equation which incorporate temporal weight parameter (ϕ), near the left boundary, for $i = 2$,

$$\begin{aligned} u\frac{\partial c}{\partial x} \approx \frac{u}{6\Delta t}[&\phi(-11c_i^{n+1} + 18c_{i+1}^{n+1} - 9c_{i+2}^{n+1} + 2c_{i+3}^{n+1}) \\ &+(1-\phi)(-11c_i^n + 18c_{i+1}^n - 9c_{i+2}^n + 2c_{i+3}^n)], \end{aligned} \tag{3.2}$$

interior nodes of the solution domain, for $i = 3, ..., M-2$,

$$\begin{aligned} u\frac{\partial c}{\partial x} \approx \frac{u}{6\Delta t}[&\phi(c_{i-2}^{n+1} - 6c_{i-1}^{n+1} + 3c_i^{n+1} + 2c_{i+1}^{n+1}) \\ &+(1-\phi)(c_{i-2}^n - 6c_{i-1}^n + 3c_i^n + 2c_{i+1}^n)], \end{aligned} \tag{3.3}$$

near right boundary, for $i = M-1$

$$\begin{aligned} u\frac{\partial c}{\partial x} \approx \frac{u}{6\Delta t}[&\phi(-2c_{i-3}^{n+1} + 9c_{i-2}^{n+1} - 18c_{i-1}^{n+1} + 11c_i^{n+1}) \\ &+(1-\phi)(-2c_{i-3}^n + 9c_{i-2}^n - 18c_{i-1}^n + 11c_i^n)], \end{aligned} \tag{3.4}$$

and to approximate the diffusive term by using central-difference scheme,

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{D}{(\Delta x^2)}[c_{i-1}^n - 2c_i^n + c_{i+1}^n]. \tag{3.5}$$

We can assumable each term by substituting Eqs.(3.1-3.5) into Eq.(2.1), we obtain the computed solution near left boundary, for $i = 2$,

$$\begin{aligned} c_i^{n+1} = ((1 - K\Delta t)c_i^n - &\frac{1}{6}Cr[\phi(18c_{i+1}^{n+1} - 9c_{i+2}^{n+1} + 2c_{i+3}^{n+1}) \\ &+ (1-\phi)(-11c_i^n + 18c_{i+1}^n - 9c_{i+2}^n + 2c_{i+3}^n)] \\ &+ \frac{Cr}{Pe}[c_{i-1}^n - 2c_i^n + c_{i+1}^n])/(1 - \frac{11}{6}Cr\phi). \end{aligned} \tag{3.6}$$

Interior nodes of the solution domain, for $i = 3, ..., M-2$,

$$\begin{aligned} c_i^{n+1} = ((1 - K\Delta t)c_i^n - &\frac{1}{6}Cr[\phi(c_{i-2}^{n+1} - 6c_{i-1}^{n+1} + 2c_{i+1}^{n+1}) \\ &+ (1-\phi)(c_{i-2}^n - 6c_{i-1}^n + 3c_i^n + 2c_{i+1}^n)] \\ &+ \frac{Cr}{Pe}[c_{i-1}^n - 2c_i^n + c_{i+1}^n])/(1 + \frac{1}{2}Cr\phi). \end{aligned} \tag{3.7}$$

Near the right boundary, for $i = M-1$,

$$\begin{aligned}c_i^{n+1} = ((1-K\Delta t)c_i^n &- \frac{1}{6}Cr[\phi(-2c_{i-3}^{n+1} + 9c_{i-2}^{n+1} - 18c_{i-1}^{n+1}) \\ &+ (1-\phi)(-2c_{i-3}^n + 9c_{i-2}^n - 18c_{i-1}^n + 11c_i^n)] \\ &+ \frac{Cr}{Pe}[c_{i-1}^n - 2c_i^n + c_{i+1}^n])/(1 + \frac{11}{6}Cr\phi).\end{aligned} \tag{3.8}$$

where $Cr = \frac{u\Delta t}{\Delta x}$ is Courant number (dimensionless), $Pe = \frac{u\Delta x}{D}$ is Peclet number (dimensionless) and $\phi \in \{0, 0.5, 1\}$.

3.2. The Modified Siemieniuch-Gladwell Implicit Scheme

The modified Siemieniuch-Gladwell technique for solving the one-dimensional advection diffusion reaction Eq.(2.1) following:

$$\begin{aligned}\frac{\partial c}{\partial t} \approx &\left(\frac{2\frac{Cr}{Pe} - Cr}{4}\right)\left(\frac{c_{i-1}^{n+1} - c_{i-1}^n}{\Delta t}\right) + \left(\frac{2 - 2\frac{Cr}{Pe} + Cr}{2}\right)\left(\frac{c_i^{n+1} - c_i^n}{\Delta t}\right) \\ &+ \left(\frac{2\frac{Cr}{Pe} - Cr}{4}\right)\left(\frac{c_{i+1}^{n+1} - c_{i+1}^n}{\Delta t}\right),\end{aligned} \tag{3.9}$$

$$\frac{\partial c}{\partial x} \approx \left(\frac{c_{i+1}^n - c_{i-1}^n}{4\Delta x}\right) + \left(\frac{c_{i+1}^{n+1} - c_{i-1}^{n+1})}{4\Delta x}\right), \tag{3.10}$$

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{1}{2}\left(\frac{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}}{(\Delta x)^2}\right) + \frac{1}{2}\left(\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n)}{(\Delta x)^2}\right), \tag{3.11}$$

substituting Eqs.(3.9-3.11) into Eq.(2.1), we have

$$\begin{aligned}-Crc_{i-1}^{n+1} + (2 + Pe)\,c_i^{n+1} = &\left(2\frac{Cr}{Pe}\right)c_{i-1}^n + \left(2 - 4\frac{Cr}{Pe} + Pe - 2K\Delta\right)c_i^n \\ &+ \left(2\frac{Cr}{Pe} - Pe\right)c_{i+1}^n,\end{aligned} \tag{3.12}$$

for $i = 1, 2, ..., M-1$.

4. Numerical Experiments

Example 4.1. The analytical solution to the one-dimensional advection-diffusion in a region bounded $0 \le x \le 1$ is taken from [16] and given,

$$c(x,t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}}\exp\left[-\frac{(x + 0.5 - t)^2}{(0.00125 + 0.004t)}\right], \tag{4.1}$$

the initial condition

$$c(x,0) = \exp\left[-\frac{(x+0.5)^2}{0.00125}\right], \tag{4.2}$$

and the boundary conditions

$$c(0,t) = \frac{0.025}{\sqrt{0.000625+0.02t}}\exp\left[-\frac{(0.5-t)^2}{(0.00125+0.004t)}\right], \tag{4.3}$$

$$c(1,t) = \frac{0.025}{\sqrt{0.000625+0.02t}}\exp\left[-\frac{(1.5-t)^2}{(0.00125+0.004t)}\right]. \tag{4.4}$$

In the analysis conducted in this study the various parameters used are $D = 0.01$ m^2/s, $u = 1$ m/s, meshes the stream into 50 elements with the space step and time step are $\Delta x = 0.02$ m and $\Delta t = 0.002$ s, respectively. Using a third order finite difference scheme Eqs.(3.6-3.8) and the modified Siemieniuch-Gladwell method Eq.(3.12) to obtain the pollutant concentration $c(x,t)$ in each point at all time on a uniform flow stream. As can see from Eqs.(3.6-3.8), $\phi = 0$ the formula corresponding to the explicit expansion of the advective term, $\phi = 1$ the formula corresponding to the explicit expansion and $\phi = 0.5$ the formula corresponding to the Crank-Nicolson scheme. The approximation of pollutant concentrations c of all schemes are shown in Table 1- Table 4. The comparison of approximated solutions of an explicit, an implicit, the Crank-Nicolson schemes, the modified Siemieniuch-Gladwell with advection diffusion reaction are shown in Fig. 2.

Table 1. The computed pollutant concentrations $c(x,t)$ (kg/m^3) when K = 0.01

	The concentrations at T=1 s						
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0184	0.1392	0.1827	0.1410	0.0143	0.0004
Implicit	0.0004	0.0179	0.1151	0.1459	0.1193	0.0222	0.0004
Crank-Nicolson	0.0004	0.0182	0.1267	0.1632	0.1300	0.0188	0.0004
Siemieniuch-Gladwell	0.0004	0.0194	0.1387	0.1733	0.1335	0.0207	0.0004

Table 2. The computed pollutant concentrations $c(x,t)$ (kg/m^3) when K = 0.1

	The concentrations at T=1 s						
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0194	0.1386	0.1733	0.1334	0.0207	0.0004
Implicit	0.0004	0.0194	0.1386	0.1733	0.1334	0.0207	0.0004
Crank-Nicolson	0.0004	0.0194	0.1386	0.1733	0.1334	0.0207	0.0004
Siemieniuch-Gladwell	0.0004	0.0189	0.1327	0.1650	0.1265	0.0195	0.0004

TABLE 3. The computed pollutant concentrations $c(x,t)$ (kg/m^3) when K = 0.5

	The concentrations at T=1 s						
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0161	0.1119	0.1430	0.1081	0.0107	0.0004
Implicit	0.0004	0.0156	0.0928	0.1144	0.0915	0.0165	0.0004
Crank-Nicolson	0.0004	0.0159	0.1020	0.1279	0.0997	0.0140	0.0004
Siemieniuch-Gladwell	0.0004	0.0170	0.1114	0.1356	0.1023	0.0154	0.0004

TABLE 4. The computed pollutant concentrations $c(x,t)$ (kg/m^3) when K = 1

	The concentrations at T=1 s						
Solution technique	0.00	0.20	0.40	0.50	0.60	0.80	1.00
Explicit	0.0004	0.0140	0.0902	0.1121	0.0830	0.0080	0.0004
Implicit	0.0004	0.0136	0.0748	0.0898	0.0703	0.0122	0.0004
Crank-Nicolson	0.0004	0.0138	0.0822	0.1003	0.0765	0.0104	0.0004
Siemieniuch-Gladwell	0.0004	0.0148	0.0896	0.1062	0.0785	0.0115	0.0004

Example 4.2. The analytical solution to the one-dimensional advection-diffusion equation of a Gaussian pulse of unit height, centred at $x_0 = 1$ in a region bounded $0 \leq x \leq 9$ is taken from [17] and given,

$$c(x,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(x-x_0-ut)^2}{D(4t+1)}\right], \tag{4.5}$$

the initial condition

$$c(x,0) = \exp\left[-\frac{(x-x_0)^2}{D}\right], \tag{4.6}$$

and the boundary conditions

$$c(0,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(-1-ut)^2}{D(4t+1)}\right], \tag{4.7}$$

$$c(1,t) = \frac{1}{\sqrt{4t+1}} \exp\left[-\frac{(8-ut)^2}{D(4t+1)}\right]. \tag{4.8}$$

The values of the various parameters used $D = 0.005$ m^2/s, $u = 0.8$ m/s, meshes the stream into 450 elements with the space step and time step are $\Delta x = 0.02$ m and $\Delta t = 0.002$ s, respectively. The approximation of pollutant concentrations c of all schemes are comparison,the solution are obtain an explicit, an implicit, the Crank-Nicolson schemes and the modified Siemieniuch-Gladwell with advection diffusion reaction are shown in Fig. 3.

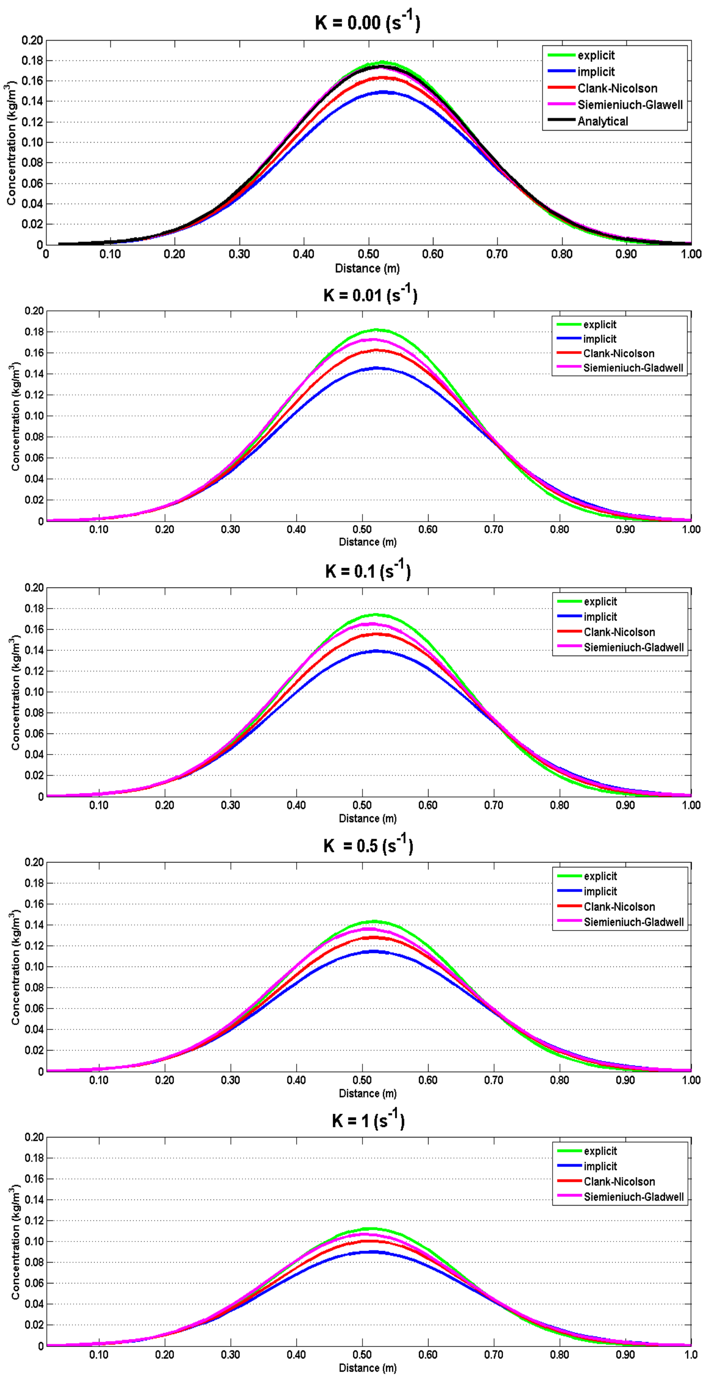

FIGURE 2. Comparison of numerical solutions techniques at $T = 1\ s$ for all $o \leq x \leq 1$ which K are varied 0.00, 0.01, 0.1, 0.5 and 1, respectively.

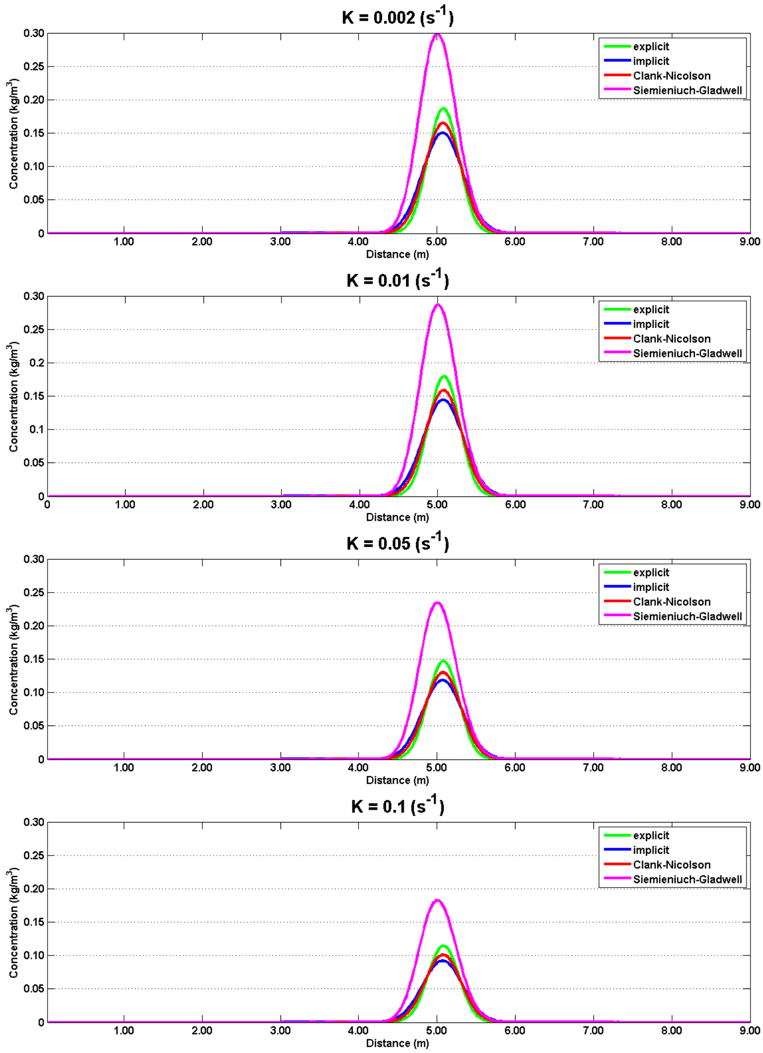

FIGURE 3. Comparison of numerical solutions techniques at $T = 1$ s for all $o \leq x \leq 9$ which K are varied 0.002, 0.01, 0.05 and 0.1, respectively.

5. Discussion and Conclusion

The one-dimensional equation advection-diffusion-reaction can be used to describe the concentration of contaminants within a uniform canal of water. In this study the cross sectional average of pollutant concentration is called for each point in the flat bottom. Finite difference approaches are developed for the one-dimensional model of water quality. Comparison is made of the approximate solution and exact solution to the ideal problem. It turns out that, by illustrated examples, the numerical computations give good agreement solutions.

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References

[1] R. Anguelov, J.M.S. Lubuma, S.K. Mahudu, Qualitatively stable finite difference schemes for advection-reaction equations, J. Comput. Appl. Math. 158 (2003) 19–30.

[2] H.V. Kojouharov, B.M. Chen, Nonstandard Methods for Advection-Diffusion Reaction Equations, World Scientific Publishing, Singapore, 2000.

[3] R.E. Mickens, Analysis of a finite-difference scheme for a linear advection-diffusion reaction equation, J. Sound Vib. 236 (2000) 901–903.

[4] K. Mukherje, S. Natesan, Parameter-uniform hybrid numerical scheme for time-dependent convection-dominated initial-boundary-value problems, Computing 84 (2009) 209–230.

[5] V.A. Titarev, E.F. Toro, High-order ADER schemes for scalar advection-reaction-diffusion equations, CFD Journal 12 (2003) 1–6.

[6] E.F. Toro, V.A. Titarev, ADER: Towards arbitrary-order non-oscillatory schemes for advection-diffusion-reaction, In Proc. 8th National Conference on Computational Fluid Dynamics, E-Land, Taiwan, August 18-20, 2001, (2001) 8–23.

[7] J.Y. Chen, C.H. Ko, S. Bhattacharjee, M. Elimelech, Role of spatial distribution of porous medium surface charge heterogeneity in colloid transport, Colloids Surf. A Physicochem. Eng. Asp. 191 (2001) 3–15.

[8] G. Li, C.R. Jackson, Simple, accurate, and efficient revisions to MacCormack and Saulyev schemes: high Peclet numbers, Appl. Math. Comput. 186 (2007) 610–622.

[9] E.M. O'Loughlin, K.H. Bowmer, Dilution and decay of aquatic herbicides in flowing channels, J. Hydrol. 26 (1975) 217–235.

[10] M. Dehghan, Numerical schemes for one-dimensional parabolic equations with non-standard initial condition, Appl. Math. Comput. 147 (2004) 321–331.

[11] A.I. Stamou, Improving the numerical modeling of river water quality by using high order difference schemes, Water Res. 26 (1992) 1563–1570.

[12] N. Pochai, A numerical computation of a non-dimensional form of stream water quality model with hydrodynamic advection-dispersion-reaction equations, Nonlinear Analysis: Hybrid Systems 3 (2009) 666–673.

[13] M. Benito, H. Chen-Charpentire, V. Kojouharov, An unconditionally positivity preserving scheme for advection-diffusion reaction equations, Math. Comput. Modelling 57 (2013) 2177–2185.

[14] P. Samalerk, N. Pochai, Numerical simulation of a one-dimensional water-quality model in a stream using a Saulyev technique with quadratic interpolated initial-boundary conditions, Abstr. Appl. Anal. 2018 (2018) 1–7.

[15] P. Samalerk, N. Pochai, A Saulyev explicit scheme for an one-dimensional advection-diffusion-reaction equation in an opened uniform flow stream, Thai J. Math. 18 (2020) 677–687.

[16] M. Dehghan, Weighted finite difference techniques for one dimensional advection-diffusion equation, Appl. Math. Comput. 147 (2004) 307–319.

[17] S. Sankaranarayanan, N.J. Shankar, H.F. Cheong, Three-dimensional finite difference model for transport of conservative pollutants, Ocean Eng. 25 (1998) 425–442.