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Evaluation of Appropriate Advective Transport Function for One-Dimensional Pollutant Simulation in Rivers

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ABSTRACT: Water quality prediction is a valuable tool for pollutant control in aquatic environments. A river system is selected and one-dimensional flow is assumed for the simulation of pollutant transport in this paper. Advective and diffusive terms of transport equation are considered separately. Different functions of advective transport are proposed and applied for a specified velocity on the discrete cells along the river and compared with each other. Abilities and flexibilities of these proposed functions are investigated and the compatible one is determined for the point source pollutant transport in the channel. Fluctuations (Maximum content of negative concentrations), tolerances (Maximum interval of negative concentrations) and attenuation (Decreasing peak of the pollutant distribution) are selected for this purpose. Quick and the proposed functions including trigonometric, simple exponential, symmetric exponential and quadratic exponential of advective transport are selected for the comparison. Results show that during the simulation period (times up to 100 seconds and times more than 100 seconds), for the estimation of attenuation, the peak of the pollutant distribution and the elimination of fluctuations and the tolerances, the proposed symmetric exponential and quadratic exponential functions of advective transport perform better than other numerical methods and presented functions. Also for all these scales both of quadratic exponential and symmetric exponential functions act similarly, therefore they can be used frequently for the simulation of pollutant transport in rivers without creating negative concentration. Moreover, simple exponential function and quick method identically predict the peak of pollutant chemograph at each downstream point.

Key words: Pollutant, Advection, Channel, Exponential Function, Trigonometric Function

INTRODUCTION

Numerical modeling of pollutant transport in water flow of river systems are mainly studied based on the one-dimensional transport equation concerning advection, diffusion and source/sink terms. The numerical solution is compared with the analytical solution in most of these studies. Some one-dimensional models were applied to a river system using higher order numerical scheme for scalar transport (Glass and Rodi 1982; Schoellhamer and Jobson 1986). Nonlinear pollutant transport, reaction and turbulent diffusion in rivers and streams were studied (Ames 1988; Yoshioka and Unami 2013). Bench mark examples and case studies were selected for the verification and calibration of some models which used for the pollutant transport in aquatic systems (Li and Duffy 2012; Schmalle and Rehmann 2014). Zones of stagnant water well mixing were affected on the advective and diffusive transport in a river system (Weitbrecht *et al*. 2003; Schmalle and Rehmann 2014). Versatility and stability of numerical accurate methods for salute transport in open channel were compared with each other (Yoshioka and Unami 2013; Falconer and Liu 1988). The impact of flow and pollution characteristics on the behavior of the lag coefficient in rivers surveyed. The conclusions showed that the lag coefficient along the river is strongly influenced by flow velocity along the river caused by the water power stations (Vankuik 1994). Zoppou and Knight (1997) suggested the analytical solution for advection-diffusion equations with spatially variable coefficients written in conservative and non-conservative forms. Results show that non-conservative forms of the equations can be yield exact solutions. A few studies performed by observed experiments in the basin like (Vanmazijk and Veling 2005). The irregularities of river banks are considered indirectly in such studies that applied a two-dimensional and a three-dimensional shallow water and river equation to simulate a passive pollutant transport (Cai *et al*. 2007; Kachiashvili *et al*.

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2007). The non-oscillatory behavior and accuracy of the scheme were demonstrated by the numerical results of this model. Coastal aquifers also considered to follow from the transport equations and contaminant transport. Experimentation and comparison with the numerical solution is done for verification in these studies (Ding and Peng 2009). (Ani *et al.* 2009) investigated the development, calibration and evaluation of two mathematical models for pollutant transport in a small river. Several parameters were considered for the model and calculated for similar streams. The application of impulse response curves based on the generalized moving Gaussian distribution function that derived approximations for impulse response curves based on other suitable distribution functions (Veling 2010). A specified pollutant transport simulated in the river environments and compared with the numerical solutions (Kim *et al.* 2011). Some studies considered a pulse-type point source through a medium of linear heterogeneity (Singh *et al.* 2012). The heterogeneity is identified by considering the velocity as a spatially dependent and linear function. The problem is interpolated in a finite domain in which the concentration values are to be evaluated and a Laplace integral transform technique has been used. . The practical finite analytic (PFA) method was applied to the solution of two solute transport problems: 1- One-dimensional advection–dispersion equation with reaction under advection dominated conditions, and 2- One-dimensional pure advection equation with reaction. They developed a triangular explicit PFA (EPFA) spatial-temporal computational molecule. The EPFA solutions were compared with solutions from the quadratic upwind differencing (QUICK) scheme. For both cases, the EPFA solution gives accurate results as long as the Courant (Cr) was close to one. Stability analysis shows that the EPFA molecule is always stable for high Pe number (Ardestani *et al.* 2015). Therefore each method considers the condition of the case study and the simple assumptions to close to the measurements.

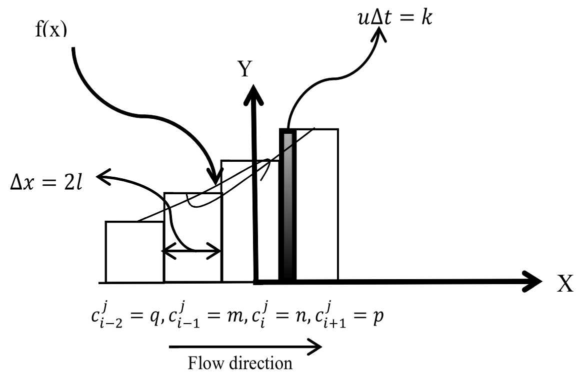

Fig. 1. The schematic pollutant transport process in the discrete length of the channel

Also a lot of researches are available for prediction of pollutant transport in river systems. Most of these studies focus on the solution method. Some of them are applied a higher dimensional model and precise discrete method. A few studies investigated this problem experimentally and compared the result with numerical solutions. In some cases the objective is the determination of some parameters of the model. A comparison with different proposed shape functions are considered for advective pollutant transport in a channel in this paper. Exponential, quadratic, trigonometric and a combination of these functions are considered separately. The elimination of negative concentrations is focused by this type of simulation. Also decreasing the peak of concentrations is compared with other numerical methods and analytical solution as well. The fluctuation of the model is calculated directly by these mentioned functions related to advective transports.

MATERIALS & METHODS

The concentration of a pollutant in a river with no turbulent flow with a specified velocity and in a one-dimensional equation is calculated as below (Hashemi *et al.* 2014):

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} + D\frac{\partial^2 c}{\partial x^2} \pm Sources/Sinks \quad (1)$$

That in this equation:

C: The concentration of pollutant [mg/l]

T: Time[s]

U: The mean velocity of the river [m/s]

X: The distance from the point source [m]

Sources/Sinks: The reaction factors of the pollutant [mg/l]

D: The dispersion coefficient [m^2/s]

For the advective transport due to the mean velocity of the river the main $\frac{\partial c}{\partial t} = u\frac{\partial c}{\partial x}$ is the important term and is calculating along the discrete distance. The distance and time intervals should be selected precisely to converge the solution of the study area. A function should be determined on the cells of discrete area for the changing in concentration. Quick method considers a quadratic function, Lax and Fromm consider linear functions and exponential or trigonometric functions could be proposed as well. A currant number as $\beta = \frac{u\Delta t}{\Delta x}$ is applied to the discrete form of equation1 and the concentration in each time and distance intervals as below:

$$C(i-2,j) = q \quad (2)$$
$$C(i-1,j) = m \quad (3)$$
$$C(i,j) = n \quad (4)$$
$$C(i+1,j) = p \quad (5)$$

That i, j are the scripts for the distance and time intervals. (Fig. 1)

Also two new parameters such as l, k are defined as $l=\frac{\Delta x}{2}$ and $k=u\Delta t$ respectively, then the constants of the quadratic function *(f(x)=ax²+bx+d),* input concentration for each cell (C_{in}) and output(C_{out}) will be calculated with a simple integration along the study area.

$$\int_{-3l}^{-l}(ax^2+bx+d)dx = 2\times m\times l \quad (6)$$
$$\int_{-l}^{l}(ax^2+bx+d)dx = 2\times n\times l \quad (7)$$
$$\int_{l}^{3l}(ax^2+bx+d)dx = 2\times p\times l \quad (8)$$

Therefore:

$$a=\frac{1}{8}\frac{p-2\times n+m}{l^2} \quad (9)$$
$$b=-\frac{1}{4}\frac{-p+m}{l} \quad (10)$$
$$d=-\frac{1}{24}p+\frac{13}{12}n-\frac{1}{24}m \quad (11)$$

and

$$c_{out}=\int_{l-k}^{l}(ax^2+bx+d)dx \quad (12)$$

$$c_{in}=\int_{-l-k}^{-l}(ax^2+bx+d)dx \quad (13)$$

Then for the quadratic (ax^2+bx+d) function the concentration of pollutant variation in each time and distance interval will be obtained as below:

$$c(i,j+1)=\left(\frac{c_{in}-c_{out}+c(i,j)*\Delta x}{\Delta x}\right) \quad (14)$$

Now the new proposed trigonometric function as *acosx+bsinx+d* or exponential function such as *(aeˣ+bx+d)* are selected and the constants and input and output concentration of pollutant for each function are calculated. Five different functions of advective transport are selected for this purpose and $C_{in}, C_{out}, C_i^{j+1}$, a, b and d are calculated for each function with MAPLE software.

A crank-nickelson method is generally used to determine the diffusion term of the transport equation (Hashemi *et al.* 2014).

An analytical solution is available for the concentrations of equation (1) as below:

$$c(x,t)=\frac{M}{A\sqrt{4\pi tD}}\exp\left(-\frac{(x-(x_0+V_x t))^2}{4Dt}\right) \quad (15)$$

In which c(x,t)= pollutant concentration at each distance and each time (mg/L); M = sudden pollutant mass at the discharge point (kg); A = area of the river cross-section *(m^2);x* = distance from point pollution source (m); *t* = time elapsed since pollution incidence in the river (s); *D* = dispersion coefficient (m^2/s); *u* = mean velocity of the river (m/s). In this equation the mean velocity,the area ofriver cross-section and dispersion coefficients are supposed constant, also it should be noted that the pollutant is point source and there is no input and output of pollution along the river.

There are many experimental methods for calculating dispersion coefficient (Seo and Cheong 1998).

In this paper Kashefipour and Falconermethod has been used to calculate the value of *D* (Kashefipour 2001, Kashefipour and Falconer 2002).

$$D_x=[7.428+1.775\left(\frac{w}{h}\right)^{0.62}\left(\frac{v}{u}\right)^{0.572}]\,hu\,\frac{v}{u} \quad (16)$$

In which *w* = width of the river section (m); *h*= water depth (m); and *v* = shear velocity (m/s). *v* is calculated using bellow equation:

$$v=\sqrt{grs} \quad (17)$$

In which *g* = acceleration gravity (9.81 *m/s²*); *R*= hydraulic radius of the river calculated as A/P [*A*= area of the river cross-section (m^2);*P* = wet perimeter of the water flow (*m*)]; and *s* = hydraulic slope of the river (m/m).

The change of concentrations in each distance and time intervals by the analytical solution are being compared with the numerical solution in most cases.A test case problem is applied with the specified boundaries for this purpose. The steady-state flow in a channel with the mean velocity equal to 10m/s is ongoing. The length of the channel is 1200 meters and a point source of pollutant is considered as below. The channel is divided to 300 cells of 4 meters distance intervals. A 100 seconds period is selected for the pollutant transport in the channel. The initial values and position of the pollutant with the peak of 1mg/l in the channel is considered as Table 1 and Fig. 2.

RESULTS & DISCUSSION

The normal test case problem that is described above is selected to be solved with the different numerical and analytical solutions of pollutant transport in the channel and compared with each other (Li and Duffy 2012; Schmalle and Rehmann 2014). Attenuation (decreasing peak of the pollutant distribution),

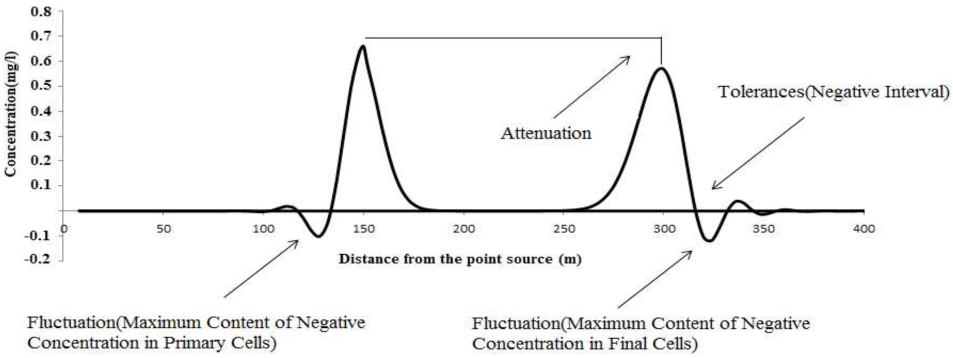

Fig. 3. Three different scales for the pollutant transport in the channel

fluctuation (Maximum negative concentration) and tolerances (Maximum interval of negative concentrations) as shown in Fig.3 are chosen for this purpose.

Quick and new presented exponential and trigonometric functions for advective transport are applied for the advective transport of the problem. For the Quick method, the maximum negative concentrations are appeared in the primary and final cells of the pollutant distribution are respectively $-6.12\times10^{-3}$and -5.93×10^{-3} just 15 seconds after the transportation (Table 2). The maximum negative concentrations decrease with the time in both primary and final cells and the rate of decreasing is the same.

The negative concentration in primary cells of pollutant distribution increases from 16 meters to 28 meters and the negative concentration in final cells increases from 20 meters to 32 meters 100 seconds after pollution entrance and is shown in the Table 3.So the negative interval increases for the primary and final cells of pollutant distribution and the rate of increasing is approximately constant. The attenuation is smooth for the Quick method as it is shown in the Fig. 4.The peak of pollutant chemograph reaches from 1mg/l to 0.23077mg/l after 100 seconds of transport. This should be compared with the analytical solution of transport equation with a point source pollutant in the channels. The attenuation of negative concentrations is also specified in Fig. 4 .The maximum decreasing rate of the peak is 0.502316mg/l and belongs to the time shows 15 seconds after the start of the transport and the peak of concentration reaches to the 0.497684mg/l in this time. For the proposed trigonometric function ($f(x) = a \times \cos(x) + b \times \sin(x) + d$) the negative concentrations are appeared in the primary cells of pollutant distribution. The fluctuations of concentrations for this part of the simulation are more than other functions (Table 4).

No negative concentration is obtained for the final cells and the maximum contents of negative concentration are more than the Quick method. This content is -0.0203mg/l directly 15 seconds after the transportation and increase to -0.0931mg/l after 100 seconds. The negative interval is a long distance for this method and covers 124 meters of the channel length after 100 seconds of transportation (Table 5).The attenuation is more than other functions in the trigonometric advective function. The peaklevel of the pollutant distribution reaches to 0.128mg/l after 15 seconds and decreases slowly to 0.0489mg/l after 100 seconds of simulation (Fig. 5). One of the exponential functions for example simple exponential ($f(x) = a\,e^{x} + b\,x + d$) is chosen for the

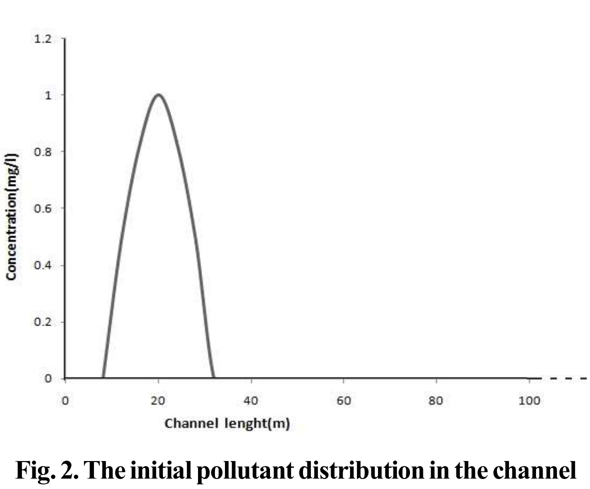

Fig. 2. The initial pollutant distribution in the channel

Table 1. The initial values of the problem

Parameter	Value	unit
A	1	m^2
w	5	m
h	0.2	m
s	0.0025	m/m
u	10	m/s
initial injection concentration	1	mg/l
channel length	1200	m
Δx	0.5	m
Δt	0.1	s

Table 2. The maximum negative concentration in the primary and final cells of pollutant distribution (Quick)

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Maximum negative concentration in primary cells(mg/l)	-6.12×10^{-3}	-2.25×10^{-3}	-1.03×10^{-3}	-5.25×10^{-4}	-2.67×10^{-4}	-1.51×10^{-4}	-9.93×10^{-5}
Maximum negative concentration in final cells(mg/l)	-5.93×10^{-3}	-2.51×10^{-3}	-1.34×10^{-3}	-7.62×10^{-4}	-4.36×10^{-4}	-2.74×10^{-4}	-2.024×10^{-4}

Table 3. The negative interval with time increasing (Quick)

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Negative concentration in primary cells(m)	16	19	22	24	26	27	28
Negative concentration in final cells(m)	20	23	26	28	30	31	32

Table 4. The maximum negative concentration of the trigonometric function in the primary and final cells of pollutant distribution

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Maximum negative concentration in primary cells(mg/l)	-0.0203	-0.0213	-0.0232	-0.0296	-0.0417	-0.0615	-0.0931
Maximum negative concentration in final cells(mg/l)	-----	-----	-----	-----	-----	-----	-----

Table 5. The negative interval with time increasing for the trigonometric function

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Negative concentration in primary cells(m)	28	50	64	82	95	111	124
Negative concentration in final cells(m)	-----	-----	-----	-----	-----	-----	-----

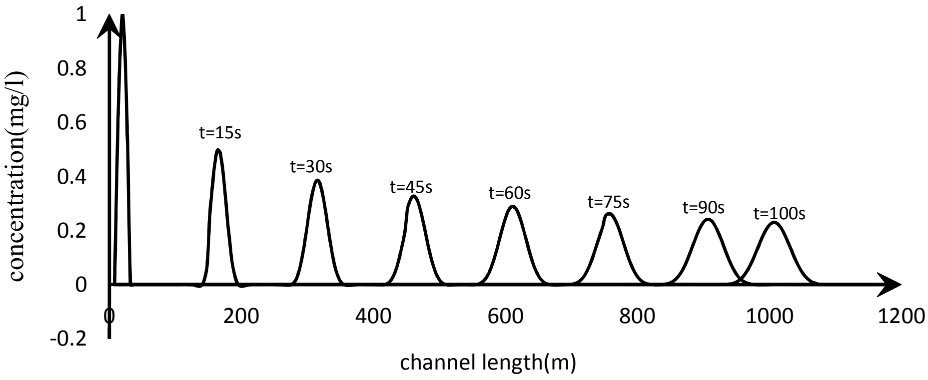

Fig. 4. The concentration of pollutant transport in the channel with the Quick method

comparison with the above functions of advective transport. As it is mentioned before the analytical solution of the transport equation is an exponential function (Eq.15). For the simple exponential function, no negative concentration is appeared in the primary cells of pollutant distribution (Table6). The value of this maximum negative concentration is -0.0861mg/l directly 15 seconds after the start of the transportation and decreases to -0.03mg/l in the final cells of pollutant distribution after 100 seconds. The negative interval for this type of advective function increases with the time increasing but the negative interval does not elongate like the trigonometric function that is described above. The negative interval is 36 meters just 15 seconds after the simulation and increases smoothly to 58 meters after 100 seconds and the rate of this increasing is decreases with the time increasing for this type of advective function. The rate of increasing of negative interval of the simple exponential function is similar to the Quick method.

The attenuation is more similar to the Quick method for the simple exponential function of advective transport. The peak of pollutant is 0.441206 mg/l just 15 seconds after the transportation and reaches to 0.208 mg/l after 100 seconds of transportation. (Fig. 6)

New exponential functions including symmetric exponential ($f(x) = a\,e^{x} + b\,e^{-x} + d$) and quadratic exponential ($f(x) = ae^{x^2} + b\,e^{x} + d$) are proposed in this paper for the comparison of different functions of advective transport. No negative concentrations are appeared for the primary and final cells of pollutant distribution. The negative interval is not available on the pollutant distribution as well. Therefore for the elimination of fluctuations the symmetric exponential and quadratic exponential functions perform more effective than other numerical methods and proposed functions. Also it is observed that symmetric exponential and quadratic exponential functions and analytical solution accurately predict the peak of pollutant chemograph at each downstream point. Thus to display the attenuation of these two types of functions the peak of pollutant distribution is compared with the analytical solution of transport equation (Table 8). As it is specified in the table 8 the simple exponential is a more effective performance in compare with the Quick method. The attenuation is approximately close to the Quick method but negative concentrations exist. Therefore for the phenomena that the negative concentrations should be eliminated, and the peak of pollutant chemograph must be well estimated the symmetric and quadratic exponential functions are better than the other advective functions (Fig. 7). During the simulation period for the elimination of fluctuation, tolerances and prediction of attenuation, the peak of the pollutant chemograph, the proposed symmetric exponential and quadratic exponential functions of advective transport, perform better than other numerical methods and other proposed functions.

Also the results are very close to analytical solution, thus these proposed functions could be used for the simulation of pollutant transport in rivers. Also for the times after 100 second, the trigonometric function is not capable to predict the pollutant transport and no convergence is occurred. Quick method eliminates the negative concentrations, but the simple exponential function does not eliminate the negative concentrations in times after 100 second. Moreover simple exponential function and quick method similarly predict the peak of pollutant distribution at each downstream point (Table 9).

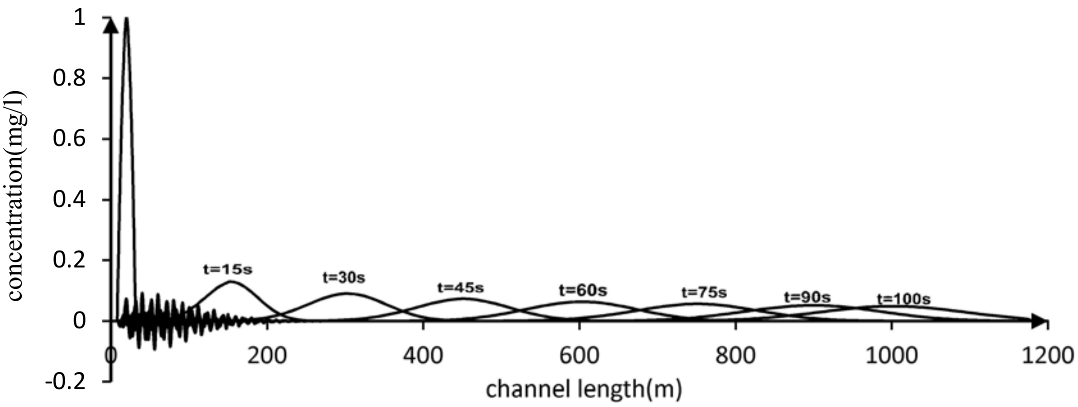

Fig. 5. The concentration of pollutant transport in the channel with the trigonometric function

Table 6. The maximum negative concentration in the primary and final cells of pollutant distribution (Simple exponential)

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Maximum Negative concentration in Primary cells(mg/l)	——	——	——	——	——	——	——
Maximum Negative concentration in Final cells(mg/l)	-0.0861	-0.0657	-0.0528	-0.0441	-0.038	-0.033	-0.030

Table 7. The negative interval with time increasing (Simple exponential)

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Negative concentration in primary cells(m)	-----	-----	-----	-----	-----	-----	-----
Negative concentration in final cells(m)	36	43	48	51	54	56	58

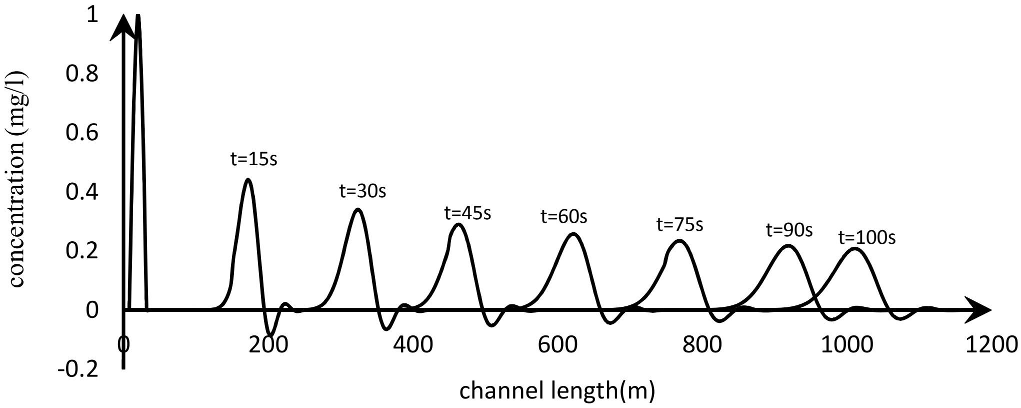

Fig. 6. The concentration of pollutant transport in the channel with the simple exponential function

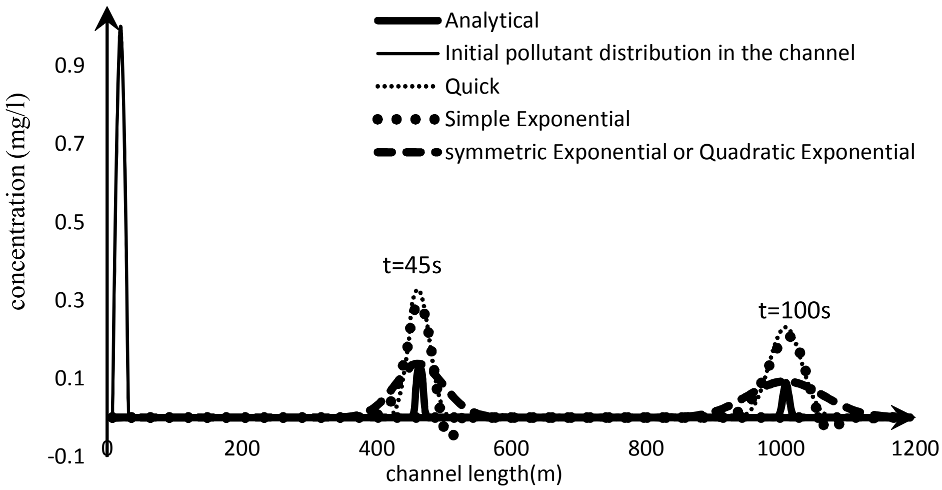

Fig. 7. The comparison of simple exponential and quadratic exponential functions with the analytical solution and Quick method

Table 8. The content of the peak of the pollutant distribution in compare with the analytical solution

Time(s)	T=15	T=30	T=45	T=60	T=75	T=90	T=100
Quick method	0.497684	0.386088	0.326615	0.29	0.262162	0.242035	0.23077
Trigonometric	0.128	0.090183	0.073422	0.063578	0.056659	0.051678	0.048948
Simple Exponential	0.441206	0.340245	0.289	0.257	0.235	0.217	0.208
Symmetric Exponential	0.235791	0.168057	0.137513	0.119261	0.10673	0.097491	0.09251
Quadratic Exponential	0.238791	0.169057	0.138513	0.119861	0.10773	0.098491	0.09291
Analytical	0.230329	0.162868	0.132981	0.115163	0.103006	0.094032	0.089206

CONCLUSIONS

A comparison for the different types of advective transport is investigated in this study. For this purpose fluctuations (Maximum content of negative concentrations), tolerances (Negative interval) and the attenuation (Decreasing peak) for the pollutant distribution are selected. A test case problem in which a pollutant distribution is available with the peak of 1mg/l in a channel is considered. The length of the channel is 1200 meters that is divided to 300 cells of 4 meters distance intervals. A one-dimensional flow with the velocity equal to 10 m/s and the diffusion coefficient equal to 0.1m^2/s is considered. Quick, with four different function including trigonometric, simple exponential, symmetric exponential and quadratic exponential of advective transport are selected and compared with each other and with the analytical solution of transport equation. A separate diffusion term is solved with the Crank-Nickelson method. Some of the functions provide fluctuations in primary cells of pollutant distribution and others in the final cells. For the elimination of negative concentrations and estimation of the peak of the pollut-

Table 9. The content of the peak of the pollutant distribution in compare with the analytical solution (Times more than 100 seconds)

Time(s)	T=100	T=900	T=1800
Quick method	0.23077	0.082089	0.052853
Trigonometric	0.048948	No Convergence	No Convergence
Simple Exponential	0.208	0.0787009	0.049362
Symmetric Exponential	0.09251	0.049031	0.029226
Quadratic Exponential	0.09291	0.050649	0.030065
Analytical	0.089206	0.051942	0.034104

ant distribution the proposed symmetric exponential and quadratic exponential functions have more effective performance and their results are more similar to the analytical solution of transport equation. Also for the peak of the pollutant distribution, the simple exponential function of advective transport is close to the Quick method. Moreover the trigonometric function is not a suitable function of advective transport for the elimination of negative intervals and even for the prediction of the peak of the pollutant distribution.

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