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Space-Time and Motion to Advection-Diffusion Equation

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Abstract

We are concerned with the study the differential equation problem of space-time and motion for the case of advection-diffusion equation. We derive the advection-diffusion equation from the conservation of mass, where this can be represented by the substance flow in and flow out through the medium. In this case, the concentration of substance and rate of flow of substance in a medium are smooth functions which is useful to generate advection-diffusion equation. A special case of the advection-diffusion equation and numerical results are also given in this paper. We use explicit and implicit finite differences method for numerical results implemented in MATLAB.
Keywords: advection-diffusion; space-time; motion; finite difference method.

Abstrak

Kami tertarik untuk mempelajari masalah persamaan diferensial ruang-waktu, dan gerak untuk kasus persamaan adveksi-difusi. Kita menurunkan persamaan adveksi-difusi dari kekekalan massa, di mana hal ini dapat diwakili oleh aliran zat yang masuk dan keluar melalui media. Dalam hal ini konsentrasi zat dan laju aliran zat dalam suatu medium merupakan fungsi halus yang berguna untuk menghasilkan persamaan adveksi-difusi. Sebuah kasus khusus persamaan adveksi-difusi dan hasil numerik juga diberikan dalam makalah ini. Kami menggunakan metode beda hingga explisit dan implisit untuk hasil numerik yang diimplementasikan dalam MATLAB.
Kata kunci: *adveksi-difusi; ruang-waktu; gerak; metode beda hingga.*

1. INTRODUCTION

Space-time and motion have been widely studied by researchers for linear, non-linear, and quasilinear cases. Z. Erich [2] classified the linear second order of partial differential equations into three types according to the criteria of discriminant sign, they are hyperbolic, parabolic, and elliptic type, where for each type respectively has criteria of discriminant sign (more than), (equal to), and (less than) zero. Moreover, the example for all those three types are respectively wave equation, diffusion equation, and Laplace's equation. In this paper, we focus on the advection-diffusion equation and the related two representative examples of advection-diffusion equation in real life. Burger's equation is one equation related to advection-diffusion with the second order nonlinear advection. R. Mickens and K. Oyedeji [6] studied the Burger's equation and the non-diffusion Fisher equation as given the following system

$$u_t + a_1\sqrt{u}u_x = D_1 u_{xx},$$

$$u_t + a_2\sqrt{u}u_x = \lambda_1\sqrt{u} - \lambda_2 u,$$

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where the above system contains square root $\sqrt{u}$ in the advection term. Other related works containing the square root $\sqrt{u}$ in advection term were studied by L. Debnath [1], P.M. Jordan [5], and G.B. Whitham [8]. The coupled of modified advection-equation, which was also so-called coupled Burger's equation, was also studied by Y. Hu [4] as shown the following system

$$u_t + \frac{1}{2}(u^2 + b^2)_x = \mu u_{xx},$$

$$b_t + (ub)_x = \nu b_{xx}.$$

The paper [4] investigated the stability of traveling waves of the above system by using the energy method under small perturbation and large wave length.

Another example of advection-diffusion equation is the model for pollution in a river and its remediation and aeration studied by Pimpunchat, et.al. [7]. The coupled reaction-diffusion-advection is shown in the following system of equations

$$\frac{\partial(AP)}{\partial t} = D_P \frac{\partial^2(AP)}{\partial x^2} - \frac{\partial(\nu AP)}{\partial x} - K_1 \frac{X}{X+k} AP + qH(x)$$

$$\frac{\partial(AX)}{\partial t} = D_X \frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(\nu AX)}{\partial x} - K_2 \frac{X}{X+k} AP + \alpha(S - X)$$

where $H(x)$ is the Heaviside function

$$H(x) = \begin{cases} 1, & x > 0 \\ 0, & otherwise \end{cases}$$

Pimpunchat, et. al. [6] were interested in the study of effect of aeration on the degradation of pollutant. The idea of that coupled equation is based on the reactions between oxygen and pollutant to produce harmless compounds.

2. MATHEMATICAL MODELING

In this paper, we consider that all motions are only in the x-axis direction. The basic equation is derived by using the principle of conservation of mass. The problem of space-time, and motion along direction of the x-axis are in our real life, such like: heat along a flat plate, and pollutant down a river. Let $\rho(x,t)$ be the concentration of the substance and $q(x,t)$ be flow rate in space and time of x and t. Moreover, $q \geq 0$ indicates that the net flow is from left to right, and also we assume that $\rho(x,t)$ and $q(x,t)$ are smooth functions. Based on the mass conservation, there are no additions or subtractions of mass, and also change of the rate of mass in an interval of Δx for the medium.

Since $\int_x^{x+\Delta x} \rho(s,t)\, ds$ is the total of mass in an interval of size Δx, then the variation in time of this quantity is given by

$$\frac{d}{dt}\int_x^{x+\Delta x} \rho(s,t)\, ds = q(x,t) - q(x+\Delta x, t) \tag{1}$$

The righthand side (1) represents the net flow in and out from left to right which across the boundary of Δx at fixed time of t. We consider that (1) is positive by assuming $q(x,t) \geq q(x+\Delta x, t)$ in an interval of Δx and (1) which indicates that the mass inside the interval of Δx is increased.

Moreover, we consider that some of substance can move into or out for the given medium with the length of Δx. This problem indicates that there is an additional source or sinks which must be calculated (for example, the heat imposed to center of flat plate is reduced because of dispersion of heat to the around flat plate, and the pollutants moving along the river from upstream to downstream, will increase because of dispersion which this pollutant is conversely proportional to the concentration of dissolved oxygen). Therefore, we consider $k(x,t)$ be the rate of change for density of source or sinks. Moreover, assume k be smooth and known function, where $k \geq 0$ and $k \leq 0$ indicates a net source and a net sink respectively.

In fact, all sources or sinks are not distributed smoothly (for example, the heat imposed to flat plate is not precisely at the center of flat plate, and the pollutants dumped into at some specific sewage outfall). Therefore, we consider the point sources or sinks be well separately.

Proposition 2.1. Let $\int_x^{x+\Delta x} k(s,t)\,ds$ be rate of change for density of source or sinks through the medium with the length of Δx. We apply this rate of change for density $k(x,t)$ to the righthand side (1) to establish the balance of mass. Then, one has

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial q(x,t)}{\partial x} + k(x,t) \tag{2}$$

Proof. It is a simple way to prove (2). We rewrite (1) by considering rate of change for density of source or sinks through the medium to get

$$\frac{d}{dt}\int_x^{x+\Delta x} \rho(s,t)\,ds = q(x,t) - q(x+\Delta x,t) + \int_x^{x+\Delta x} k(s,t)\,ds. \tag{3}$$

Noting that

$$\frac{d}{dt}\int_x^{x+\Delta x} \rho(s,t)\,ds = \int_x^{x+\Delta x} \frac{\partial \rho(s,t)}{\partial t}\,ds, \tag{4}$$

and

$$q(x,t) - q(x+\Delta x,t) = -\int_x^{x+\Delta x} \frac{\partial q(s,t)}{\partial s}\,ds \tag{5}$$

We substitute (4) and (5) into (3) to get

$$\begin{aligned}
\int_x^{x+\Delta x} \frac{\partial \rho(s,t)}{\partial t}\,ds &= -\int_x^{x+\Delta x} \frac{\partial q(s,t)}{\partial s}\,ds + \int_x^{x+\Delta x} k(s,t)\,ds \\
0 &= \int_x^{x+\Delta x} \frac{\partial \rho(s,t)}{\partial t}\,ds + \int_x^{x+\Delta x} \frac{\partial q(s,t)}{\partial s}\,ds - \int_x^{x+\Delta x} k(s,t)\,ds \\
0 &= \int_x^{x+\Delta x} \left(\frac{\partial \rho(s,t)}{\partial t} + \frac{\partial q(s,t)}{\partial s} - k(s,t)\right) ds \\
0 &= \left(\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial q(x,t)}{\partial s} - k(x,t)\right) \Delta x + o(\Delta x)
\end{aligned} \tag{6}$$

We finally divide (6) by Δx and take the limit $\Delta x \longrightarrow 0$, then we complete the proof of (2). ■

Furthermore, the negative sign of flow rate $\frac{\partial q(x,t)}{\partial x}$ in (2) is reasonable, because the flow rate through the medium Δx should be decreasing. Moreover, let q be a smooth function of ρ which is written as $q \equiv q(\rho)$, then the equation (2) becomes

$$\frac{\partial \rho}{\partial t} = -\frac{dq(x,t)}{d\rho(x,t)}\frac{\partial \rho(x,t)}{\partial x} + k(x,t), \tag{7}$$

where the equation (7) is still considered general. Noting that the term of $\frac{dq(\rho)}{d\rho}$ is typically a nonlinear function of ρ.

In the present paper, two special cases are very interesting to be studied. Firstly, for some $u(x,t)$, the case of q as a function of ρ is advection, where $q = u\rho$. We consider function of $u(x,t)$ as the velocity of the substance moving along the x-axis. For simplification of advection case, we assume that the velocity of $u(x,t)$ be constant with the constant velocity of c. Then $\frac{dq}{d\rho}$ is identical to constant velocity of c. Moreover, we can also interpret it into another way. In time of Δt, the substance moving with the distance $\Delta x = c\Delta t$, then the integration bound of (1) becomes

$$\int_x^{x+c\Delta t} \rho(s,t)\, ds \tag{8}$$

which represents all the substance moving along the x-axis during the time of Δt.

Proposition 2.2. It follows from (8), we divide it by Δt and let Δt goes to zero, then the total of mass in (8) changing along the x-axis is equal to flow rate of $q(x,t)$. Therefore (8) becomes

$$q(x,t) = \lim_{\Delta t \to 0} \frac{1}{\Delta t}\int_x^{x+c\Delta t} \rho(s,t)\, ds = c\rho(x,t) \tag{9}$$

Proof. Similarly, we can employ the same technique in Proposition 2.1, that is

$$\int_x^{x+c\Delta t} \rho(s,t)\, ds = \rho(s,t)\, \mathrm{c}\Delta t + o(\mathrm{c}\Delta t) \tag{10}$$

We further divide (10) by Δt and take the limit $\Delta t \longrightarrow 0$, then the proof of (9) is completed. ■

Secondly, for the case of q as a function of ρ is diffusion, where $q = -\nu\frac{\partial \rho}{\partial x}$ (for example, heat flow which is changing to time and space). Moreover, this heat flow is always from a higher to a lower temperature, where it is mathematically stated as follows

$$q(x,t) = -\nu\frac{\partial \rho(x,t)}{\partial x} \tag{11}$$

for a constant of proportionality of $\nu > 0$. The minus sign shows of $\frac{\partial \rho}{\partial x}$ indicates that heat imposed to the center of medium reduces at specific time t because of heat diffusion. Finally, based on the previous discussion of two cases for advection and diffusion, we substitute the advection term $q = \rho u$, and diffusion term $q = -\nu\frac{\partial \rho}{\partial x}$ into (7), then respectively we have

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial x} + k \tag{12}$$

for the advection equation, and

$$\frac{\partial\rho}{\partial t} = \nu\frac{\partial^2\rho}{\partial x^2} + k, \tag{13}$$

for diffusion equation. Combining (12) and (13), then we have the following advection-diffusion equation

$$\frac{\partial\rho}{\partial t} = \nu\frac{\partial^2\rho}{\partial x^2} - \frac{\partial(\rho u)}{\partial x} + k. \tag{14}$$

3. NUMERICAL RESULTS

In this section, we establish the numerical results of equation (14), where k is assumed to be zero for the simplicity. First, we give an example of advection-diffusion equation for case of the pollutant in the river, where u is the pollutant flow rate and ν is the dispersion of pollutant.

$$\frac{\partial\rho}{\partial t} = \nu\frac{\partial^2\rho}{\partial x^2} - u\frac{\partial\rho}{\partial x}, \qquad 0 \le x \le 80,\ 0 \le t \le 60 \tag{15}$$

We discretize (15) by using the finite difference method by explicit, central differences for the second derivative in space x, forward differences in time t, and backward differences for the first derivative, namely,

$$\rho_{i,j+1} - \rho_{i,j} = \frac{\nu\Delta t}{\Delta x^2}\left[\rho_{i-1,j} - 2\rho_{i,j} + \rho_{i+1,j}\right] - \frac{u\Delta t}{\Delta x}\left[\rho_{i,j} - \rho_{i-1,j}\right]$$

By grouping the same terms for j and $j+1$, then

$$\rho_{i,j+1} = \rho_{i,j} + \frac{\nu\Delta t}{\Delta x^2}\left[\rho_{i-1,j} - 2\rho_{i,j} + \rho_{i+1,j}\right] - \frac{u\Delta t}{\Delta x}\left[\rho_{i,j} - \rho_{i-1,j}\right]$$

The analytical solution of (15) is the Gaussian distribution given as

$$\rho(x,t) = \mathrm{h}\cdot\exp\left(-\frac{x-20-ut}{20}\right), \tag{16}$$

where h = 1 is the height of Gaussian distribution and (16) is a modified version of analytical solution given in [3]. Then, we present the following initial condition and boundary conditions of (16), respectively

$$\rho(x,t=0) = \exp\left(-\frac{x-20}{20}\right) \tag{17}$$

and

$$\rho(x=0,t) = \rho(x=80,t) = 0 \tag{18}$$

The numerical results are given as follows with the various of the rate of pollutant flow (u) and dispersion of pollutant (ν).

Table 1. Comparison results for the change of concentration of pollutant for various the rate of pollutant flow and dispersion of pollutant.

Time (t)	Rate of pollutant flow (u)	$\rho(x,t)$ at the top and fixed value $v = 2.5$	Time (t)	Dispersion of pollutant (v)	$\rho(x,t)$ at the top and fixed value $u = 2.5$
10.6667	0.5	0.3844	19.2000	0.5	0.4727
9.2903	1.5	0.3890	11.5200	1.5	0.4097
8.2286	2.5	0.3964	8.2286	2.5	0.3964
7.3846	3.5	0.4040	6.4000	3.5	0.3912
6.6977	4.5	0.4126	5.2364	4.5	0.3883
6.1277	5.5	0.4205	4.4308	5.5	0.3873
5.6471	6.5	0.4290	3.8400	6.5	0.3864
5.2364	7.5	0.4366	3.3882	7.5	0.3856
4.8814	8.5	0.4448	3.0316	8.5	0.3850

Figure 1 to Figure 4 represents the changes of the concentration of the pollutant in the river from the initial time to final time. It can be seen that, the more increase the time is, the more declined the graph is for each time t. This indicates that, there is diffusion of pollutant while the pollutant is moving along the river for time t. Figure 1 and Figure 2 show the changes of the concentration of the pollutant for various rate of pollutant flow and fixed dispersion of pollutant from the initial time to final time. It can be concluded that the higher the rate of pollutant flow is, the higher the value of $\rho(x,t)$ at the top is. Moreover, Figure 3 and Figure 4 show the changes of the concentration of the pollutant for various dispersion of pollutant and fixed rate of pollutant flow from the initial time to final time. These results are inversely proportional to Figure 1 and Figure 2 that the higher the dispersion of pollutant is, the lower the value of $\rho(x,t)$ at the top is. All the numerical results for various the rate of pollutant flow and dispersion of pollutant are presented in Table 1.

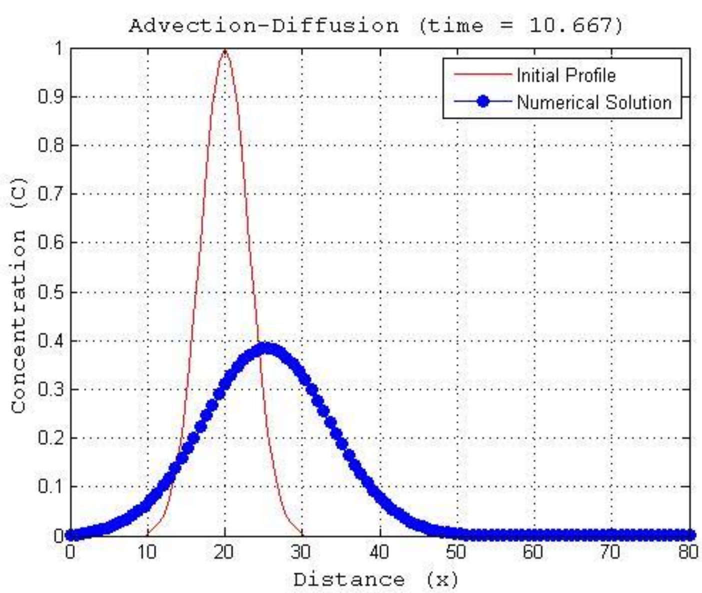

Figure 1. Rate of pollutant flow ($u = 0.5$)

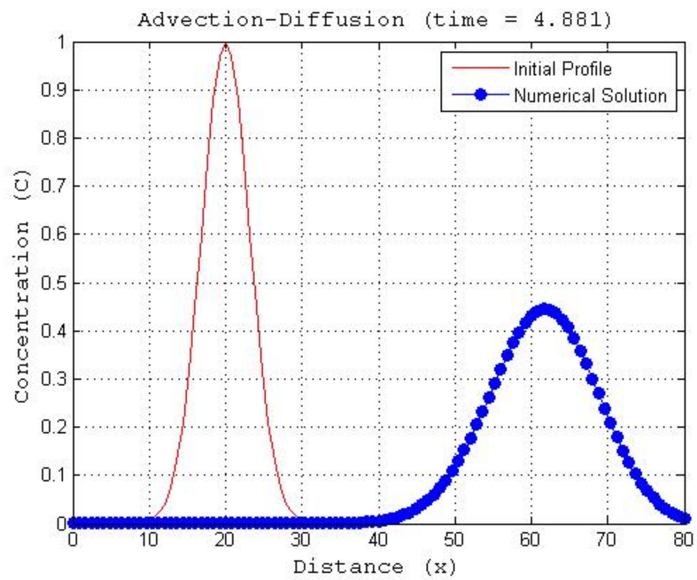

Figure 2. Rate of pollutant flow ($u = 8.5$)

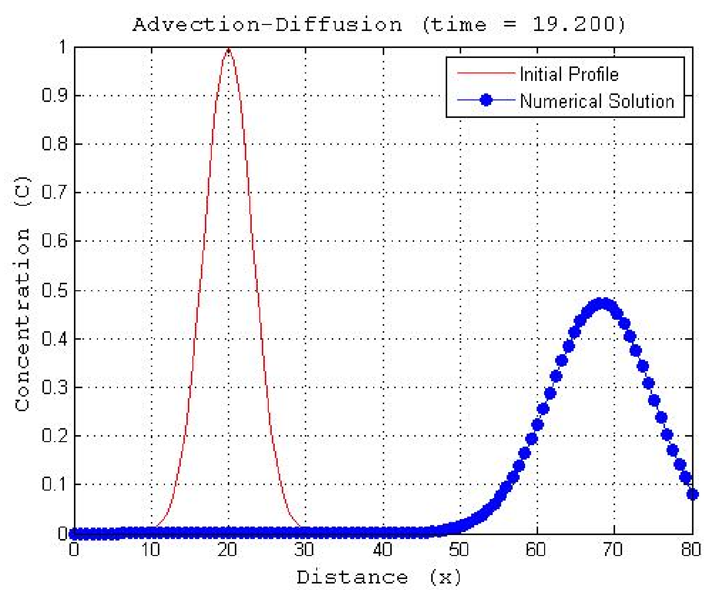

Figure 3. Dispersion of pollutant ($\nu = 0.5$)

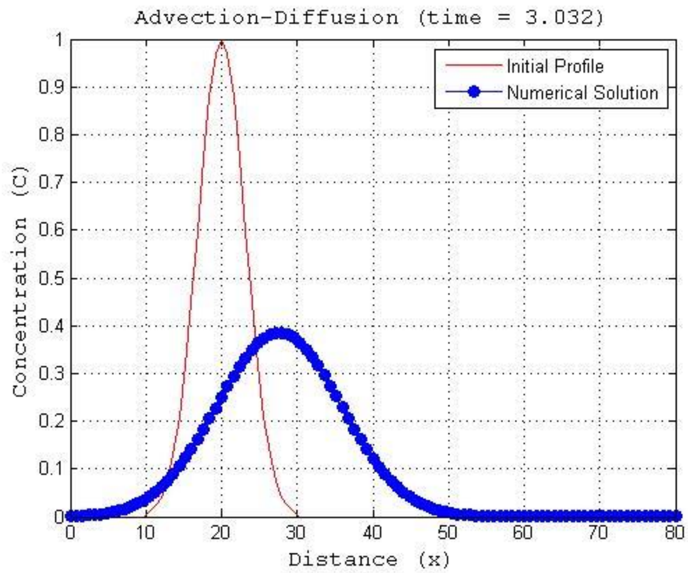

Figure 4. Dispersion of pollutant ($v = 8.5$)

In the real life, the first condition, the increasing pollutant flow rate for all the time does not give the significant effect for reduction in pollutant. This is due to the constant dispersion of pollutant when the pollutant moves along the river. There is the possibility of other pollutants addition along the river, causing more pollutants. The second condition give the significant effect for reduction in pollutant though the pollutant move along the river with the constant flow rate. This can happen because the higher dispersion of pollutant for all the time along the river. The other example of advection is for case of pollutant and dissolved oxygen in upstream and downstream of the river as shown the following steady state equation with zero dispersion

$$0 = -\frac{\partial\left(vAP_s(x,t)\right)}{\partial x} + ZP_s(x,t), \tag{19}$$
$$0 = -\frac{\partial\left(vAX_s(x,t)\right)}{\partial x} + \alpha S - X_s(x,t),$$

where P_s is concentration of pollutant, X_s is concentration of dissolved oxygen, $A = 2$ is the cross-section area of the river, $v = 0.7$ is the water velocity in the x-direction, $Z = 1$ is the mass transfer of solid to the water of river, $\alpha = 0.5$ is the mass transfer of oxygen from air to water, and $S = 0.2$ is the saturated oxygen concentration. The boundary conditions of (19) are given as follows

$$(P_s, X_s)(0) = \left(\frac{q}{kA}, S + \frac{q}{kA}\right) \tag{20}$$

where $k = 2$ is the degradation rate and $q = 0.098$ is the rate of pollutant addition along the river. Then, we use the upwind method to solve (19) numerically

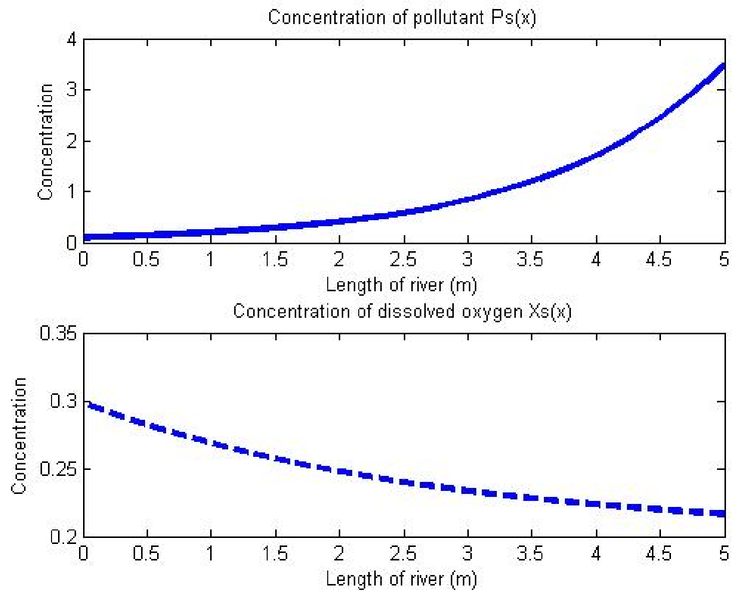

Figure 5. Concentration of pollutant and dissolved oxygen.

Figure 5 represents concentration pollutant and dissolved oxygen which is moving from the point $x = 0$ meter to $x = 5$ meter. It appears that at the initial distance ($x = 0$), the level of pollution (solid line) in the upstream is small enough. However, in downstream, the pollutant appears that the level of pollution concentration (solid line) is increasing. However, the rate of pollution concentration (solid line) is inversely proportional to the rate of dissolved oxygen concentration (dashed line). This is because in the upstream area the level of concentration of pollutant is small, so the dissolved oxygen concentration is still high. The concentration of pollutant is higher when the concentration of dissolved oxygen is lower, so that the dissolved oxygen concentration decreases, this is due to the greater use of dissolved oxygen for the pollution oxidation process.

4. CONCLUSIONS

Based on the numerical results and two examples of case for advection-diffusion equation, we conclude that it is possible to study this space-time and motion problem from the simple real life through the problem of pollutant in the river, and dissolved oxygen in the river. We further can make a simulation by using explicit, and upwind method, and then interpret the simulation results into the real life whether it makes sense or not.

The first problem states the correlation between the rate of pollutant flow and dispersion of pollutant where the higher rate of pollutant flow cause the higher concentration of pollutant, and the higher dispersion of pollutant cause the lower concentration of pollutant. The second problem studies the correlation between concentration of pollutant and concentration of dissolved oxygen, where the concentration of dissolved oxygen is inversely proportional to the concentration of pollutant. The concentration of dissolved oxygen is higher than the concentration of pollutant in the upstream, and the concentration of dissolved oxygen is lower than the concentration of pollutant in the upstream.

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