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Unravelling the Influence of Advection and Diffusion on the Spatial and Temporal Evolution of Pollutant Concentration

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ABSTRACT

The spatial distribution and temporal evolution of pollutant concentration are complex phenomena. Advection and diffusion are the primary drivers influencing the dynamic of pollutant concentrations. This paper aims to investigate and elucidate the roles of advection and diffusion on pollutant concentration's spatial and temporal evolution in a one-dimensional domain. The finite element method (FEM) is used to solve the governing equation numerically. The underlying concepts of FEM hand-to-hand with MATLAB software were presented. The simulation study revealed that advection and diffusion uniquely impact the system's dynamic. Advection, driven by the bulk movement of water, leads to rapid and long-range transport of pollutants, while diffusion, driven by random molecular motion, causes more gradual dispersion. The interplay between these processes is a critical determinant in understanding the overall behaviour of pollutant concentrations over time and space.

1. Introduction

The advection-diffusion equation is a type of partial differential equation (PDE) that poses a significant role in modelling transport phenomena. Some applications of the advection-diffusion are to model the transportation in shallow porewater [1], a reactive rock [2], a porous media [3], a turbulent pipe flow [4], open-channel flows [5], and street canyon [6]. In other studies, Jamil and Wang discussed the PBE-advection-diffusion model for the enzymatic hydrolysis process [6-13]. In 2019, Azimi and Jamil presented diffusion-reaction and coupled diffusion-reaction-advection models for ethanol production systems via fermentation [14,15]. Their result shows that the diffusion was insignificant on the whole ethanol production system but is contrary to the advection.

The advection-diffusion equation can be used to model the spatial evolution of a system. The action of particles moving from one location to another is driven by two terms: advection and diffusion. Those two terms act differently, where advection goes following the streamline or mean flow while diffusion disperses the particles to another place regardless of the stream direction [16].

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In other words, advection is typically drifted by fluid flow movement. Diffusion, conversely, is drifted by the molecular motion where particles move from areas of high concentration to low concentration. Diffusion does not require the movement of fluid flow to move; instead, it relies on the kinetic energy of particles [22].

Since analytical solutions do not exist for most practical engineering problems, one always resorts to numerical methods to obtain the approximate solution. The most commonly used numerical methods include Finite Difference Method (FDM), Finite Volume Method (FVM), Boundary Element Method (BEM), Meshfree Methods, Collocation Method, and Finite Element Method (FEM). For example, Dehghan [17] solved the three-dimensional advection-diffusion equation using FDM. Abidin and Misro [18] presented the solution to the heat transfer problem on two-dimensional irregular geometry by applying FEM and recommended exploring mesh refinement and optimization. In their study, the comparison of triangular and rectangular mesh in the heat transfer problem showed a good agreement. Mojtabi and Deville [19] solved a one-dimensional advection-diffusion equation analytically and numerically using FEM. They found the analytical solution harder to evaluate if the advection term becomes dominant. From all of those methods, solving the advection-diffusion problem using FEM will be our main interest. FEM is the most stable numerical scheme compared to FDM and FVM [20]. Using FEM, the domain is discretized into smaller elements. A system of algebraic equations is formulated for each element called a local stiffness matrix. The overall solution is then obtained by assembling all the local solutions throughout the domain.

The spatial distribution and temporal evolution of pollutant concentration in a fluid flow are complex phenomena. This study area has greatly interested environmental scientists, policymakers, and practitioners involved in pollution control and risk assessment. There is a lack of comprehensive knowledge of the significant role and interplay of advection and diffusion in shaping the spatially and timely pollution concentration pattern. With a clear understanding of how advection and diffusion contribute to pollutant distribution, it is easier to design effective management strategies and sustainable solutions to mitigate water pollution. Therefore, this study aims to investigate and elucidate the roles of advection and diffusion on pollutant concentration's spatial and temporal evolution in a one-dimensional domain. The work is organized as follows. In Section 2, the methodology of this research was presented. Besides, the essential step using FEM, including pre-processing, post-processing, and processing, were also discussed in this section. Section 3 is devoted to the results and discussion of the simulation study. Lastly, in Section 4, the conclusion is discussed.

2. Methodology

Consider an unsteady linear advection-diffusion equation given by the following relation

$$\frac{\partial U}{\partial t} - v\frac{\partial^2 U}{\partial x^2} + \alpha\frac{\partial U}{\partial x} = 0, \quad -1 \le x \le 1, \quad t > 0 \tag{1}$$

where U is the concentration of the pollutant at point *x* at time *t*, α is the advection coefficient (velocity of water flow), and v is the diffusion coefficient. The second term on the left-hand side of Eq. (1) describes the loss or gain of the concentration due to diffusion, while the third term denotes the influence of advection on the concentration. This partial differential equation (PDE) problem is subjected to homogeneous Dirichlet boundary conditions

$$U(-1,t) = U(1,t) = 0,$$

and the initial condition

$$U(x,0) = -\sin \pi x + 1.$$

The main factors affecting pollutant concentration distribution in the domain were diffusion and advection velocity. We take into account the fact that particles move through space due to diffusion and advection. The advection-diffusion problems involve a double discretization process: space discretization and time discretization. In this paper, space discretization is performed by the Finite Element Method (FEM). Various methods can be employed to trace the temporal evolution of the solution of the advection-diffusion problem. The Crank-Nicolson Scheme will be employed for time discretization.

A usual practise in the FEM of time-dependent problems consists of discretizing first with respect to the spatial variables, thus obtaining of coupled first-order ODE (with respect to time). Then, it remains to integrate the first-order DE system forward in time to trace the temporal evolution of the solution. The steps of using the FEM were summarized in the flow chart, as shown in Figure 1. There were three major stages, namely pre-processing, processing, and post-processing.

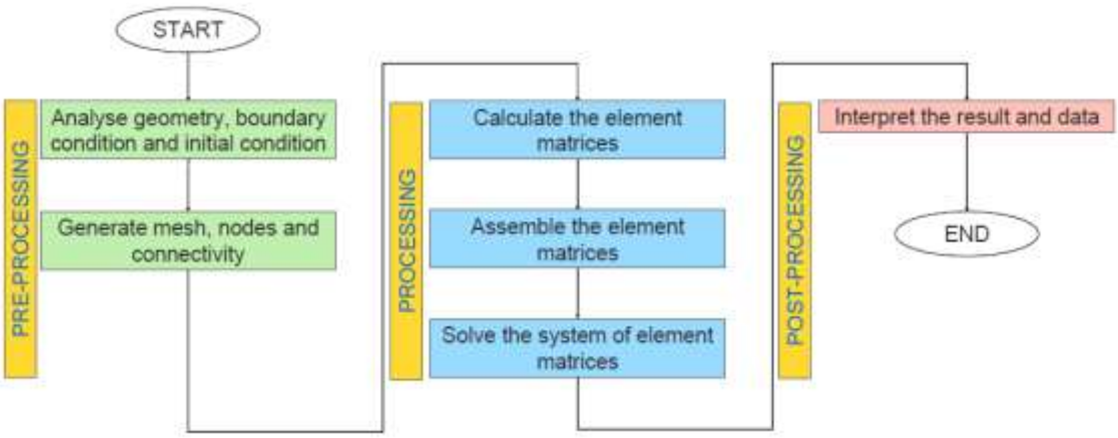

Fig. 1. Flow chart for finite element method

2.1 Pre-Processing

The FEM starts with the pre-processing step. It involves the setup of geometry, boundary condition and initial condition of the problem. The geometry is a one-dimensional space $-1 \le x \le 1$ with a total length of 2. The boundary condition and initial condition were given directly in the previous part. Then, the process is continued with the generation of mesh, nodes and connectivity. For simplification, suppose the domain is discretized equally into three elements in such a way that every element consists of two nodes as shown in Figure 2.

Fig. 2. Three elements and four nodes

Hence, the total number of nodes for that mesh is equal to 4. The connection of all nodes and elements is tabulated in Table 1. For element 2, the connected nodes are 2 and 3.

Table 1
Elements and nodes connectivity

Element	1st node	2nd node
1	1	2
2	2	3
3	3	4

Here in this study, we consider 100 finite elements which every element consists of two nodes yielding 101 nodes. The source code of MATLAB for solving the stated advection-diffusion problem in the pre-processing stage is given as follows.

```
%% Geometry, boundary and initial conditions
x_i=-1;                                        % Initial point (x=0)
x_f=1;                                        % Final point (x=1)
L=x_f-x_i;                                    % Domain length
alpha=1;                                      % Convection velocity
v = 1/(10*pi);

% Initial condition
u_0_fun=@(x) -sin(pi*x);       % Initial condition

% Boundary condition
bound_cond_fun={@(t) 0,@(t) 0};         % Boundary conditions

%% Meshing
Nx = 100;                                       % Number of finite
elements
ndof = Nx + 1;

% Elemental length
h=L/Nx;                                  % Length of a finite element
```

2.2 Processing

The most crucial step in FEM is the processing stage. The weak form is governed, and a system of algebraic equations is derived. The resulting equations were computed and transformed into a matrix system. The steps are described and listed in the following.

i. Calculate the element matrices
First, one needs to calculate the element matrices. In this study, we consider linear element which has two nodes per element. Suppose the trial function is a polynomial function

$$U = a_1 + a_2 x$$

and the Galerkin Weighted Residual Method equation is

$$U(x,t) = N_1(x)u_1(t) + N_2(x)u_2(t)$$

where $N_1(x)$, $N_2(x)$ are shape functions and $u_1(t)$, $u_2(t)$ are the degree of freedom. By performing evaluation at the nodes, one can derive the shape functions are follows.

$N_1(x) = \dfrac{x_2 - x}{x_2 - x_1}$ and $N_2(x) = \dfrac{x - x_1}{x_2 - x_1}$.

By referring to the strong form equation in Eq. (1), next, we write the weak form of the governing equation using the Galerkin residual method. By applying residual to Eq. (1), we obtained

$$\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} - v \frac{\partial^2 u}{\partial x^2} = R \tag{2}$$

where *R* is the residual error. Eq. (2) is multiplied with a set of weight function i.e. the shape functions. The residual error should not exist; hence the integration of that multiplication should be set to zero. The governing equation yields a weak form given by

$$\int_0^L N_i \left(\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} - v \frac{\partial^2 u}{\partial x^2} \right) dx = 0$$

or

$$\int_{x_1}^{x_2} \left(N_i \frac{\partial (N_1 u_1 + N_2 u_2)}{\partial t} + \alpha N_i \frac{\partial (N_1 u_1 + N_2 u_2)}{\partial x} - N_i v \frac{\partial^2 (N_1 u_1 + N_2 u_2)}{\partial x^2} \right) dx = 0 .$$

By using integration by parts,

$$\int_{x_1}^{x_2} \left(N_i N_j \frac{\partial u_j}{\partial t} + \alpha N_i \frac{\partial N_j}{\partial x} u_j + v \frac{dN_i}{dx} \frac{dN_j}{dx} u_j \right) dx = 0$$

Hence, the matrix system for one element is given by

$$\begin{bmatrix} \int_{x_1}^{x_2} N_1 N_1 \, dx & \int_{x_1}^{x_2} N_1 N_2 \, dx \\ \int_{x_1}^{x_2} N_2 N_1 \, dx & \int_{x_1}^{x_2} N_2 N_2 \, dx \end{bmatrix} \begin{bmatrix} \frac{\partial u_1}{\partial t} \\ \frac{\partial u_2}{\partial t} \end{bmatrix} + \begin{bmatrix} \alpha \int_{x_1}^{x_2} N_1 \frac{\partial N_1}{\partial x} dx & \alpha \int_{x_1}^{x_2} N_1 \frac{\partial N_2}{\partial x} dx \\ \alpha \int_{x_1}^{x_2} N_2 \frac{\partial N_1}{\partial x} dx & \alpha \int_{x_1}^{x_2} N_2 \frac{\partial N_2}{\partial x} dx \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$
$$+ \begin{bmatrix} v \int_{x_1}^{x_2} \frac{\partial N_1}{\partial x} \frac{\partial N_1}{\partial x} dx & v \int_{x_1}^{x_2} \frac{\partial N_1}{\partial x} \frac{\partial N_2}{\partial x} dx \\ v \int_{x_1}^{x_2} \frac{\partial N_2}{\partial x} \frac{\partial N_1}{\partial x} dx & v \int_{x_1}^{x_2} \frac{\partial N_2}{\partial x} \frac{\partial N_2}{\partial x} dx \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$[M]\{\dot{U}\}+[K]\{U\}+[D]\{U\}=0$$

$$[M]\{\dot{U}\}+([K]+[D])\{U\}=0$$

where

$$[M]=\frac{h}{6}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix},\ [K]=\frac{\alpha}{2}\begin{bmatrix}-1 & 1\\ -1 & 1\end{bmatrix},\text{ and } [D]=\frac{v}{h}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}$$

In time-dependent problems, the spatial representation provided by finite elements need to be accurately transported in time to trace the transient response. By discretizing the time derivative using Crank-Nicolson Scheme, i.e. $\theta=\frac{1}{2}$, the matrix system for one element is obtained as follows.

$$[M]\left(\frac{\{U\}_{s+1}-\{U\}_s}{\Delta t}\right)+\theta([K]+[D])\{U\}_{s+1}+(1-\theta)([K]+[D])\{U\}_s=0$$

$$[M](\{U\}_{s+1}-\{U\}_s)+\Delta t\theta([K]+[D])\{U\}_{s+1}+\Delta t(1-\theta)([K]+[D])\{U\}_s=0$$

$$([M]+\Delta t\theta([K]+[D]))\{U\}_{s+1}=[M]\{U\}_s-\Delta t(1-\theta)([K]+[D])\{U\}_s$$

$$\left([M]+\frac{\Delta t}{2}([K]+[D])\right)\{U\}_{s+1}=\left([M]-\frac{\Delta t}{2}([K]+[D])\right)\{U\}_s$$

The source code of MATLAB for the element metrics also known as local stiffness matrix is as follows.

```
% local stiffness matrix

k = alpha/2*[-1 1;
            -1 1];

m = h/6*[2 1;
            1 2];

d = v/h*[1 -1;
            -1 1];

%% Discretize time
t_i=0;                                        % Initial time
t_f=2;                                      % Final time

dt=1/10;
T=t_i:dt:t_f;                                 % Time vector
```

ii. Assemble the element matrices
Next, one needs to assemble all the element matrices according to the nodes connectivity to obtain the global matrix as coded in MATLAB software as follows.

```
% Global matrix
K = zeros(ndof,ndof);
M = zeros(ndof,ndof);
D = zeros(ndof,ndof);
U_0 = zeros(ndof,1);

for i = 1:ndof -1
          K([i i+1],[i i+1])= K([i i+1],[i i+1])+k;
          M([i i+1],[i i+1])= M([i i+1],[i i+1])+m;
          D([i i+1],[i i+1])= D([i i+1],[i i+1])+d;
end
```

iii. Solve the system of element matrices
The global matrix system in the form of

$$K_e T = R_e$$

can be solved using MATLAB programming software. By imposing the essential boundary conditions, the global matrix system can be reduced to a smaller size. The source code of MATLAB for solving the system is as follows.

```
% Solve for global
U=zeros(ndof,1);

G1 = M + dt/2*(K+D);
G2 = (M - dt/2*(K+D))*U_0;

dof_k=[1 4];
U_b = 0; % boundary condition

% boundary condition
U([1 4])= U_b;    %

%F=F-K(:,1)*U_b-K(:,4)*U_b;
G2=G2-G1(:,1)*U_b-G1(:,4)*U_b;

%Solve the matrix system
dof_u=setdiff(1:ndof,dof_k);        % node 2, 3,

%solve for U at iteration = 1
G2(dof_u) = (M(dof_u,dof_u) -
dt/2*(K(dof_u,dof_u)+D(dof_u,dof_u)))*U_0(dof_u);
U(dof_u)=G1(dof_u,dof_u)\G2(dof_u)
```

2.3 Post-Processing

The last stage in FEM is the post-processing stage which involved the interpretation of result and data. In this paper, the FEM result of the advection-diffusion problem is discussed in Section 3.

3. Results and Discussion

The advection-diffusion problem is solved numerically using FEM, which is coded in MATLAB software to assemble 100 elements from $t = 0$ s to $t = 2$ s with $\Delta t = 0.1$ in a one-dimensional domain. Then, the effect of advection and diffusion is simulated. The evolution of the pollutant concentration in the model with zero in both advection velocity and diffusion coefficient ($\alpha = 0$ and $v = 0$) is shown in Figure 3. The variation of the colour scheme and symbol in the figure is based on the times recorded at $t = 0, 0.5, 1, 2$. All the curves overlap, and it is difficult to distinguish from one to the other at different times. The profile projection is initially a sine function with a higher concentration on the left zone. As time goes by, the results show that the pollutant concentration remains at its position. It indicates that without the factor of advection or diffusion, the spatial distribution of the pollutant concentration does not change.

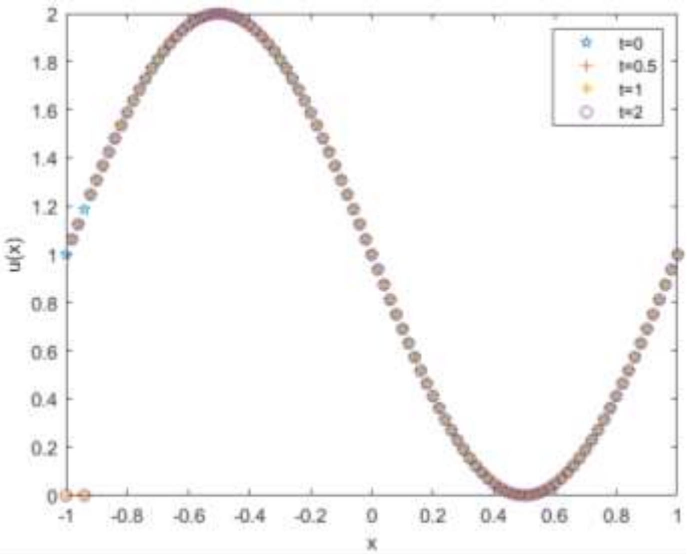

Fig. 3. The evolution of pollutant concentration with zero advection and diffusion coefficient i.e. $\alpha = 0$ and $v = 0$

Next, we consider advection in addition to diffusing through the surrounding medium. This is the case of simultaneous effects of advection and diffusion. We set $\alpha = 1$ and $v = \frac{1}{\pi}$. The evolution of the pollutant concentration is shown in Figure 4. Initially, the peak value of pollutant concentration is 2 at $x = -0.5$, and the minimum value is 0 at $x = 0.5$. The left zone originally had a higher concentration than the right area. As time goes by, the value of pollutant concentration at the right spot is more significant than that in other places, which is brought out by the presence of advection velocity. The highest concentration on the left zone decreases over time because of diffusion into the unoccupied interior of the domain. After a sufficiently long time, the highest concentration is located at the right end of the boundary due to the velocity moving the pollutant particles to the right, which is known as the advection effect.

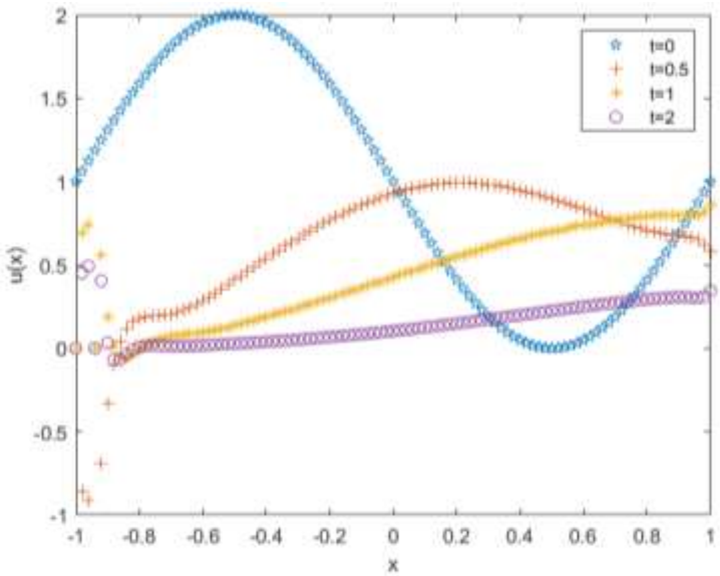

Fig. 4. The evolution of pollutant concentration for $\alpha = 1$ and $v = \frac{1}{\pi}$

In order to reveal the effect of advection on the model, simulation for $\alpha = 1$ and $v = 0$ is performed, and the spatial distribution of pollutant concentration is presented in Figure 5. The advection takes place and accelerates the movement of pollutants particles and significantly alters the spatial distribution from the initial setting. The pollutant concentration is moved to the right zone concerning time, indicating a significant contribution of advection velocity to the model. It is observed that without the diffusion factor, the peak value remains high and does not decrease during the early simulation time, as depicted in Figure 5.

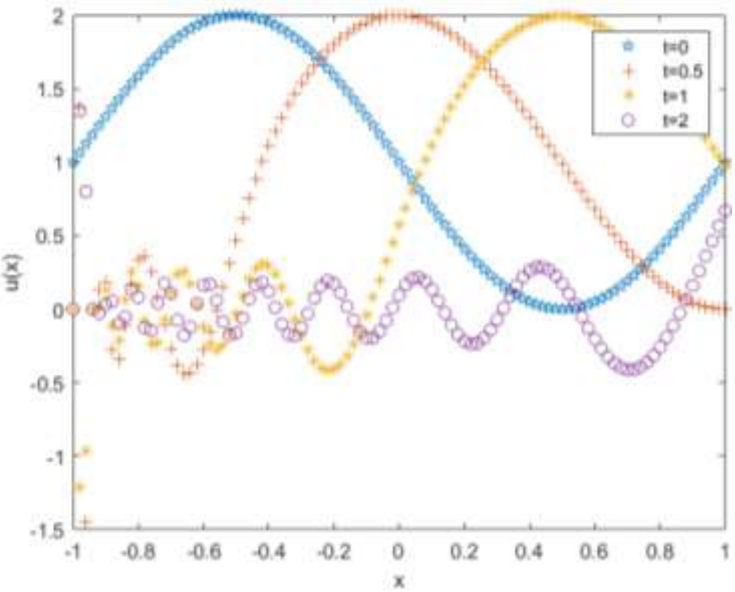

Fig. 5. The evolution of pollutant concentration for $\alpha = 1$ and $v = 0$

To elucidate the role of diffusion in the model, we set $\alpha = 0$ and $v = \frac{1}{\pi}$ for the advection and diffusion coefficients, respectively. As illustrated in Figure 6, diffusion alone can also prominently alter the pollutant concentration distribution. Initially, the pollutant particles are concentrated heterogeneously, and it is apparent from the graph that diffusion makes particles move from high to low concentration so that the domain fills up with the species over time. However, the effect of pushing the pollutant particles to the right zone is not obviously seen compared to the case in Figure 6.

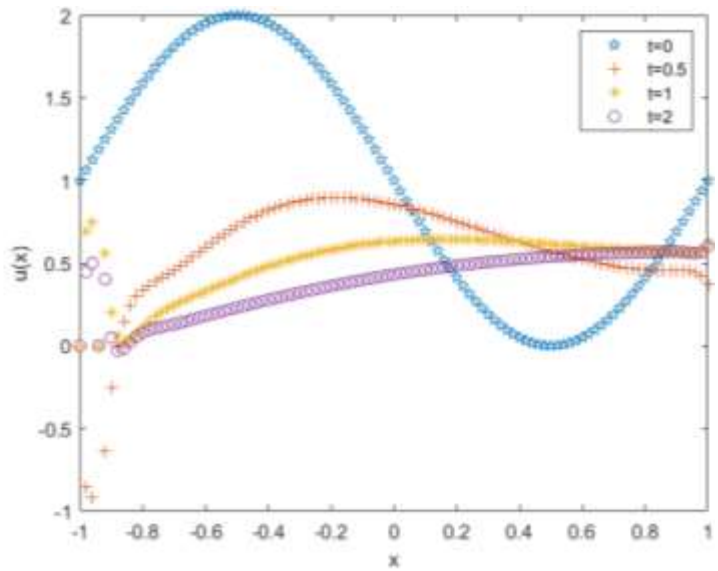

Fig. 6. The evolution of pollutant concentration for $\alpha = 0$ and $v = \frac{1}{\pi}$

The findings in this study matched with Celia *et al.,* [21], stating that the numerical solution procedures perform well when diffusion is the dominant process. However, the numerical solution exhibits nonphysical oscillations when advection is the dominant transport process. In the case of the evolution of the pollutant concentration distribution, the expected value needs to be positive or zero because the negative value of concentrations has no physical meaning (Dehghan). One of the possible solutions to avoid negative concentration is to apply an extremely fine mesh refinement. However, this approach will cost excessive computation.

The simulation study revealed that advection and diffusion are distinct mechanisms that uniquely impact the system's dynamic. Advection, driven by the bulk movement of water, leads to rapid and long-range transport of pollutants from one location to another. Through advection, the transportation of the pollutant is carried along with the moving fluid. Driven by random molecular motion, diffusion, on the other hand, causes gradual dispersion, spreading the pollutant evenly over time.

In terms of transport speed, the advection effect is much faster than diffusion, as the speed of the advection depends on the velocity of the fluid. Diffusion is a slower process where the diffusion rate depends on the concentration gradient. Advection can transport pollutants over long distances and significant spatial scales, while diffusion disperses the pollutant over short distances. Although diffusion does not transport the pollutant particles as quickly as advection, diffusion is essential for achieving homogenization and equilibrium in the system. The interplay between advection and diffusion is a critical determinant in understanding the overall behaviour of pollutant concentrations over time and space. The combination of both factors will significantly speed up the movement of particles.

4. Conclusions

In conclusion, this study delved into the intricate process of pollutant concentration dynamics within a one-dimensional domain. The investigation focused on two fundamental mechanisms: advection and diffusion. Using the finite element method (FEM) in conjunction with MATLAB software, we were able to shed light on the distinct roles played by advection and diffusion in shaping the spatial and temporal evolution of pollutant concentrations. The findings from the simulation study revealed that advection emerged as the force responsible for rapid and extensive pollutant transport, covering great distances in a relatively short period. In contrast, diffusion acted as a more deliberate dispersal mechanism, gradually spreading pollutants throughout the domain. The interplay between these two processes dictates the overall behaviour of pollutant concentrations over time and space. This study enhances the understanding of the complexities inherent in the dynamics of pollutant concentrations.

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