

Numerical Schemes to Solve Advective Contaminant Transport Problems with Linear Sorption and First Order Decay

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ABSTRACT

Hyperbolic equations are related to advection problems in which dissipative phenomena are minimal or may be considered negligible. There are a number of environmental problems involving this type of equation. This paper provides new, efficient schemes to solve problems of contaminant transport of a soluble contaminant through saturated soil under stationary flow in which reversible equilibrium controlled by sorption and irreversible decay are considered. The solution of this equation using classical methods, such as Finite Differences and Lax-Wendroff, is typically found to produce dissipation and other spurious effects that are purely numerical. The Cubic Interpolated Pseudo-particle (CIP) method is used to eliminate these numerical errors. Specifically, the CIP approach is used to provide stable numerical predictions to the advection-sorption-decay equation even in cases where the solution involves discontinuities in the concentration profile. Comparisons of the numerical predictions obtained using this method for the case of one-dimensional problems of known analytical solution show a clear superiority of the CIP approach in relation to other numerical approaches.

KEYWORDS: Contaminant transport; Advection; Linear sorption; First order decay; Numerical schemes, CIP method.

INTRODUCTION

Many problems in environmental engineering involve advection phenomena. Perhaps the best known of such problems is the transport of solutes by fluids percolating in porous media. This problem is governed by different mechanisms, including advection, hydrodynamic dispersion, sorption and decay (Freeze & Cherry, 1979; Van Genuchten, 1991; Bear & Cheng, 2010).

Among the multiple mechanisms that are relevant for the proper representation of the phenomenon, advection is the transport mechanism whose numerical implementation often leads to problems. This is because the solution to the advection process is fundamentally different than that of the hydrodynamic dispersion, sorption and decay processes. Specifically, while the latter processes tend to smooth the concentration profile, the advection process tends to maintain it and

often results in discontinuities in the concentration profile. Consequently, special attention should be paid to the implementation of numerical techniques to solve the transport equations if the advective transport dominates the problem.

Among the various transport mechanisms, advection is the one by which the solute is carried by the fluid, generally water, with or without interaction with the porous media. In problems involving advective transport without interaction with the porous media, the contamination front is often abrupt, advancing at a velocity equal to the average linear velocity (v) of the percolating fluid. In addition, the advective transport in this case does not lead to alterations in the peak concentration.

The effective percolation velocity of the fluid can be computed as the discharge velocity (defined using Darcy's law) divided by the porosity of the medium. The hydraulic conductivity of the soil is a fundamental parameter for the solute transport problem, since it quantifies the media resistance to the movement of the percolating fluid and, consequently, of the dissolved solute. Accordingly, advection represents solute transport induced by the presence of a hydraulic gradient.

Hyperbolic equations govern advective problems in which dissipative phenomena are either not present or can be considered negligible. The solution of such problems requires the knowledge of initial and boundary conditions. The general mathematical formulation of an advective problem, in one-dimensional space, is described by the following hyperbolic equation:

$$c_t + v_p \cdot c_x = 0 \quad (1)$$

where v_p is the effective percolation velocity. The independent variable c is the solute concentration, with c_x and c_t denoting the concentration derivatives in relation to distance x and time t , respectively. The term $v_p \cdot c_x$ in Eq. (1) is often referred to as the advective term.

Ultimately, Eq. (1) represents the transport of solute with concentration c for increasing distance x . Since this equation does not contain a dissipative term, c_{xx} , the solute is just transported along x , without undergoing any alteration from time t_0 to time $t_0 + \Delta t$. The absence of dissipative mechanisms implies that any discontinuity in the initial conditions should propagate to the solution at any time. Accordingly, the solution to this transport problem should admit discontinuous concentration profiles, and the numerical method adopted to solve the hyperbolic equations should be able to deal efficiently with such discontinuities.

The initial value problem, or Cauchy problem, for the advection equation involves finding a function $c(x, t)$ in the semi-space $D = \{(x, t) / t \geq 0, -\infty < x < \infty\}$, that satisfies Eq. (1) and a particular set of initial and boundary conditions. The solution to this problem is often not a continuous or sufficiently differentiable function.

This paper presents the Cubic Interpolated Pseudo-particle (CIP) method as a new tool to deal with problems involving advection processes with linear sorption and first order decay. While the CIP method has been previously used to solve other hyperbolic equations, it has never been used to solve contaminant transport problems involving both advective and decay mechanisms. Specifically, this study investigates this problem using the CIP approach to provide stable numerical predictions to the advection-sorption-decay equation. Numerical predictions obtained using this method will be compared against analytical results as well as against numerical predictions obtained using other traditional numerical schemes such as Finite Differences and Lax-Wendroff.

ADVECTIVE CONTAMINANT TRANSPORT WITH LINER SORPTION ISOTHERM AND FIRST ORDER DECAY

The mass conservation equation can be derived considering the mass balance of a contaminant moving through a one-dimensional Representative Elementary Volume (REV) in a saturated undeformable porous media (Bear, 1972), as follows:

$$-(J_A)_x = n \cdot c_t + r \quad (2)$$

where J_A is the advective mass flux of contaminant in pore fluid, with $(J_A)_x$ denoting its derivative in relation to the spatial coordinate x , n is the porosity of the soil, r is the rate of contaminant mass sink per unit volume, and t is the time.

The advective mass flux is given by:

$$J_A = v_p \cdot n \cdot c \quad (3)$$

The mass sink rate represents the sorption of the contaminant onto the soil skeleton, and it can be represented by:

$$r = \rho_d \cdot S_t \quad (4)$$

where ρ_d is the soil dry density and S is the mass of sorbed contaminant per unit mass of dry soil, with S_t denoting its derivative in relation to time t .

Combining Eqs. (3) and (4) into Eq. (2), and assuming that the soil porosity is spatially invariant, results in the one-dimensional advection transport equation with sorption:

$$-n \cdot v_p \cdot c_x = n \cdot c_t + \rho_d \cdot S_t \quad (5)$$

Applying the chain rule to Eq. (5) leads to the one-dimensional advective transport equation with reversible equilibrium controlled by sorption:

$$-n \cdot v_p \cdot c_x = (n + \rho_d \cdot S_c) \cdot c_t \quad (6)$$

Considering the case of advective transport with linear sorption, the rate of change of sorbed contaminant with respect to the contaminant concentration remains constant, as follows (Freeze & Cherry, 1979):

$$S_c = K_d \quad (7)$$

where K_d is the equilibrium partitioning coefficient of the contaminant between the fluid and solid phases.

Substituting Eq. (7) into Eq. (6) leads to the linear advective transport equation:

$$c_t + \frac{v_p}{R} \cdot c_x = 0 \quad (8)$$

with,

$$R = 1 + \frac{\rho_d K_d}{n} \quad (9)$$

where R is the retardation coefficient.

Considering the effect of a linear first-order irreversible decay, acting simultaneously with linear reversible sorption, the sink term can be rewritten as:

$$R = (n + \rho_d \cdot K_d) \cdot (c_t + \lambda \cdot c) \quad (10)$$

where λ is the rate coefficient for the first-order decay.

Combining Eqs. (3) and (10) into Eq. (2) leads to the advective transport equation with linear sorption and first order decay, as follows:

$$c_t + \frac{v_p}{R} \cdot c_x + \lambda \cdot c = 0 \quad (11)$$

ANALYTICAL SOLUTION FOR THE ADVECTIVE EQUATION WITH LINEAR SORPTION ISOTHERM AND FIRST ORDER DECAY

The analytical solution of Eq. (11) in the semi-space D, subjected to an initial condition $c(x, 0) = c_0(x)$, is given by:

$$c(x, t) = c_0 \left(x - \frac{v_p}{R} \cdot t \right) \cdot \exp(-\lambda \cdot t) \quad (12)$$

where $c_0(x)$ is a function describing the initial concentration profile for any x and $t = 0$. If the transport occurs in a finite domain (e.g. $x \in [x_L, x_R]$) and if $v_p/R > 0$, a boundary condition of the form $c(x_L, t) = c_L(t)$ must be specified, where $c_L(t)$ is a known boundary condition. In contaminant transport problems, this boundary condition specifies the concentration at the “outflow boundary”.

When the linear sorption and reactive decay are not considered, R equals 1 and λ equals 0. Consequently, the solution presented in Eq. (12) turns into:

$$c(x, t) = c_0(x - v_p t) \quad (13)$$

which is the traditional analytical solution for the advection problem.

In fact, in the absence of any other term, and for a constant effective percolation velocity v_p , it is not necessary to use numerical methods to solve this equation. Nonetheless, this problem was selected to illustrate the occurrence of unrealistic dissipative components that appear in the numerical solutions predicted when using some classical numerical methods. This problem will also allow comparison of the analytical solution to the numerical predictions obtained using the CIP method.

As an example, consider the problem of a constant wave propagating at a velocity $v_p = 1$ m/s, along x , with the initial condition given by (Fig. 1):

$$c_0(x) = \begin{cases} 0 \text{ mg/L}, & 0 \text{ m} \leq x < 1 \text{ m} \\ 0.5 \text{ mg/L}, & 1 \text{ m} \leq x \leq 2 \text{ m} \\ 0 \text{ mg/L}, & x > 2 \text{ m} \end{cases} \quad (14)$$

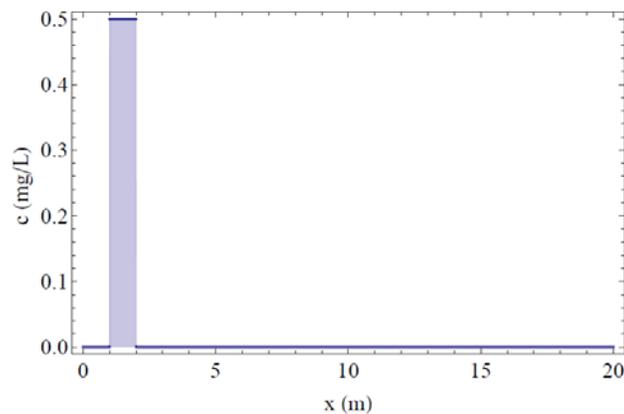


Figure 1: Initial condition ($t = 0$ s) for the advective example problems.

As the initial constant wave propagates due to the advection as the only transport mechanism, it will not suffer any dissipation or retardation (Fig. 2a). However if sorption and decay phenomena are considered (e.g. considering $R = 2$ and $\lambda = 0.1 \text{ s}^{-1}$), the initial constant wave will suffer retardation and dissipation due to these processes, as illustrated in Figs. 2(b), 2(c) and 2(d).

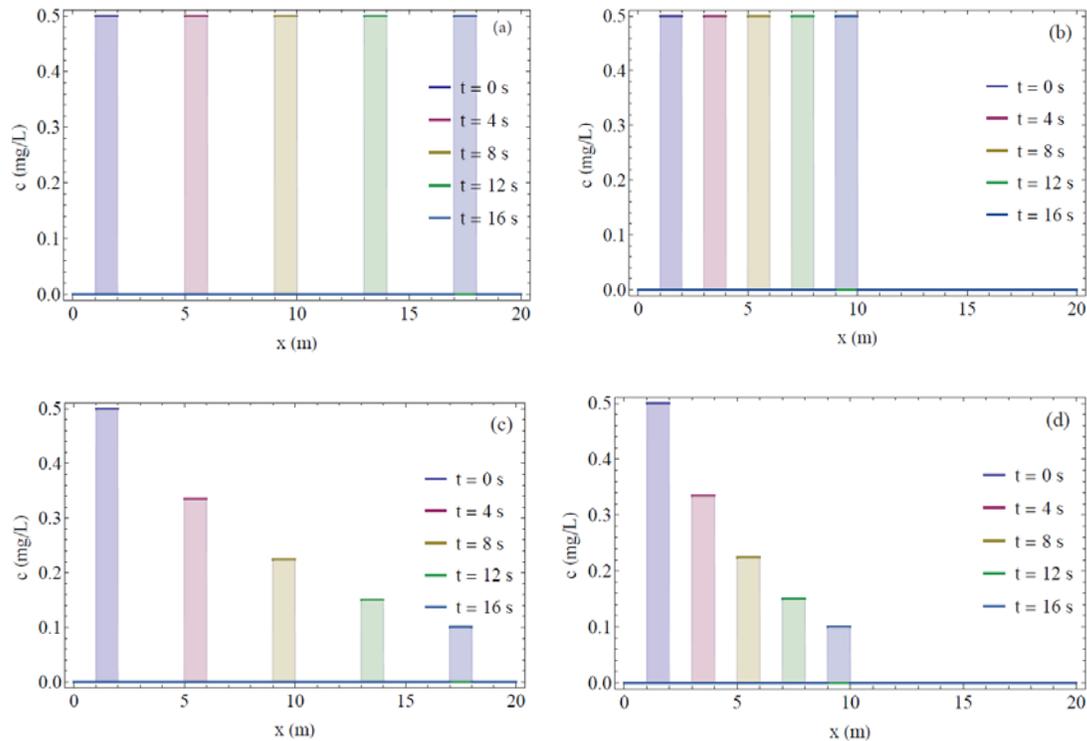


Figure 2: Analytical solutions for the advective propagation problem: (a) without sorption nor decay ($v = 1$ m/s; $R = 1$; $\lambda = 0$ s $^{-1}$), (b) without decay but with sorption ($v = 1$ m/s; $R = 2$; $\lambda = 0$ s $^{-1}$), (c) with decay but without sorption ($v = 1$ m/s; $R = 1$; $\lambda = 0.1$ s $^{-1}$), and (d) with decay and sorption ($v = 1$ m/s; $R = 2$; $\lambda = 0.1$ s $^{-1}$).

The overall solutions ($x, t, c(x,t)$), for the four cases, are also shown in the Fig. 3 using three-dimensional plots. Specifically, Fig. 3(b) allows observing the three-dimensional representation of the analytical solution of the advective phenomenon with sorption and without decay when compared with the results in Fig. 3(a), where only the advective phenomenon is observed. As can be observed, the sorption phenomenon results in a retardation processes, but it does not cause dissipations in the concentration. Fig. 3(c) allows observing the effect of the decay phenomenon, which results in a dissipation process but it does not cause retardation. Finally, Fig. 3(d) illustrates the effect of advection when both sorption and decay are relevant processes.

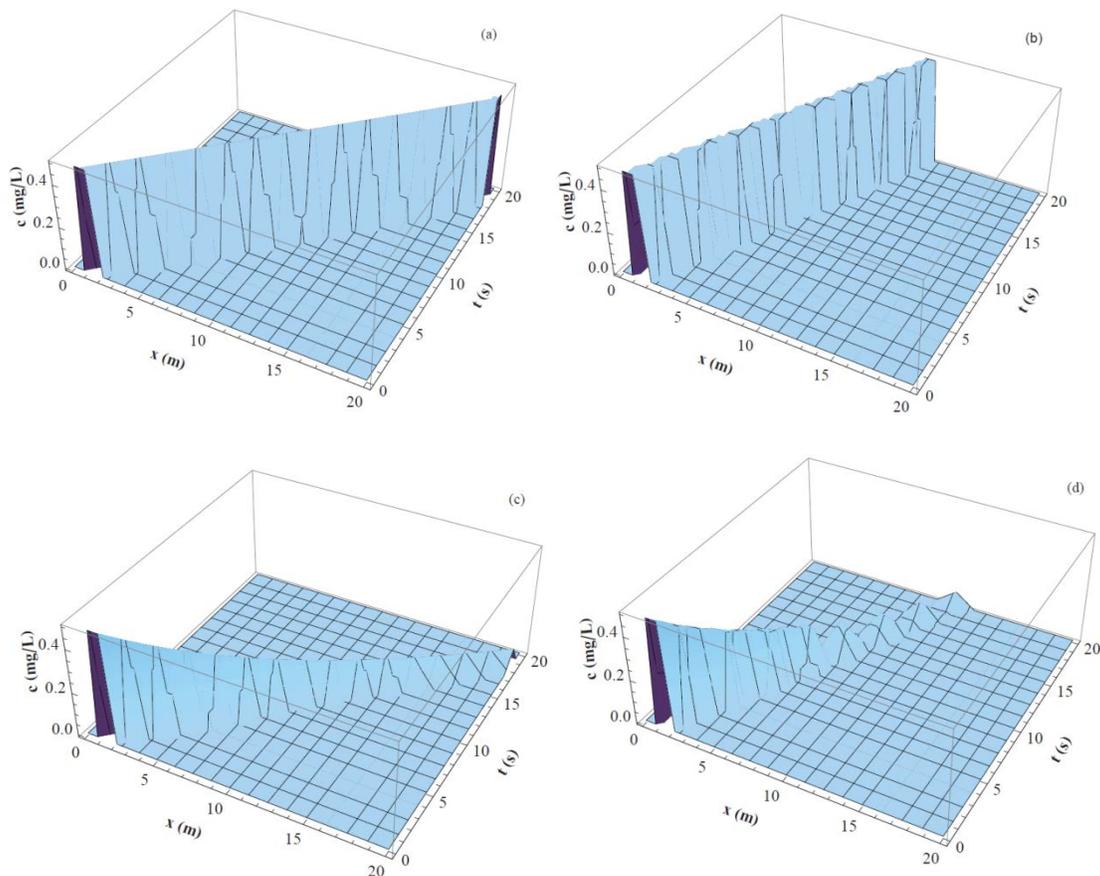


Figure 3: Three-dimensional representation of the analytical solutions for the advective propagation problem: (a) without sorption nor decay ($v = 1$ m/s; $R = 1$; $\lambda = 0$ s $^{-1}$), (b) without decay but with sorption ($v = 1$ m/s; $R = 2$; $\lambda = 0$ s $^{-1}$), (c) with decay but without sorption ($v = 1$ m/s; $R = 1$; $\lambda = 0.1$ s $^{-1}$), and (d) with decay and sorption ($v = 1$ m/s; $R = 2$; $\lambda = 0.1$ s $^{-1}$).

NUMERICAL SOLUTIONS OF ADVECTION PROBLEMS USING TRADITIONAL METHODS

As previously discusses, hyperbolic equations such as that represented by Eq. (1) involve propagation of the initial condition of the relevant variable (i.e. c) at a constant velocity that may not suffer physical dissipation mechanisms. The initial condition may present discontinuities, which in this case should propagate without showing dissipation. The solution may show erroneous dissipation trends if the problem is not adequately treated numerically. When the problem involves physical dissipation mechanisms such as those represented by Eq. (11), the numerical results could present dissipative trends that are a combination of actual physical dissipation mechanisms and erroneous numerical spurious results.

The most common numerical treatment for problems such as that represented by Eq. (1) involves adopting a forward scheme in time and a central scheme in the space domain. Despite its simplicity, the stability of this method cannot be guaranteed with a simple criterion. A more stable solution using Finite Differences may be obtained by adopting a forward scheme in time

and a backwards difference in space, leading to the following fully explicit algorithm (Xiao, 1996; Zienkiewicz & Morgan, 2006):

$$c_k^{n+1} = C_r \cdot c_{k-1}^n + (1 - C_r) \cdot c_k^n \quad (15)$$

with,

$$C_r = v_p \cdot \frac{\Delta t}{\Delta x} \quad (16)$$

where C_r is known as the Courant number and, according to von Neumann (Smith, 1985), a stability criterion can be defined when $C_r \leq 1$.

Using this numerical approach, the exact solution, $c_k^{n+1} = c_{k-1}^n$, can only be obtained when $C_r = 1$. Also, the solution at an upstream location $k-1$ of a given point k at time n , c_{k-1}^n , should be transported to the point k at time $n+1$, c_k^{n+1} , without any dissipation. While there is sufficient information to compute c_k^{n+1} without numerical instabilities in cases with $C_r < 1$, the exact solution is not predicted accurately. The profile $c(x, t)$ is similar to that observed for problems involving dissipative phenomena, although this dissipative trend in the solution is purely numerical and undesirable. Fig. 4(a) shows the numerical results for the previously discussed problem with initial conditions defined by Eq. (14) and with the exact solution being shown in Fig. 2(a). The prediction in Fig. 4(a) used a Courant number $C_r = 0.5$, with the propagation of the initial condition being shown for times $t = 4, 8, 12, 16$ s. Numerical dumping of the initial condition can be clearly noticed, with decreasing amplitudes of the constant wave as the numerical solution propagates in time.

The dissipative trend observed in Fig. 4(a) is the product of numerical errors, which should be avoided since the real problem does not involve dissipation mechanisms. Since the numerical solution should approximate better the exact solution illustrated in Fig. 2(a), a novice in the use numerical techniques may be tempted to “improve” the numerical solution by using smaller time intervals Δt . This would, in fact, resulting a decrease of the Courant number C_r and provide a significantly poorer numerical approximation. Fig. (4b) illustrates the results for the same problem and at the same times ($t = 0, 4, 8, 12, 16$ s) but using $C_r = 0.25$ (Fig. 4b). The smaller time intervals (and smaller C_r) led to more pronounced undesirable numerical results.

Another classical method to solve numerically the advective problem is that proposed by Lax & Wendroff (1960). In this case, the numerical approximation for the advection equation (Eq. (1)) is expressed as:

$$c_k^{n+1} = p_1(C_r) \cdot c_{k-1}^n + p_2(C_r) \cdot c_k^n + p_3(C_r) \cdot c_{k+1}^n \quad (17)$$

with,

$$p_1(C_r) = \frac{1}{2} \cdot C_r \cdot (C_r + 1) \quad (18)$$

$$p_2(C_r) = (1 - C_r) \cdot (1 + C_r) \quad (19)$$

$$p_3(C_r) = \frac{1}{2} \cdot C_r \cdot (C_r - 1) \quad (20)$$

where C_r is the Courant number and $p_k(C_r)$ are the polynomials given in Eqs. (18), (19), (20) and illustrated in Fig. 5.

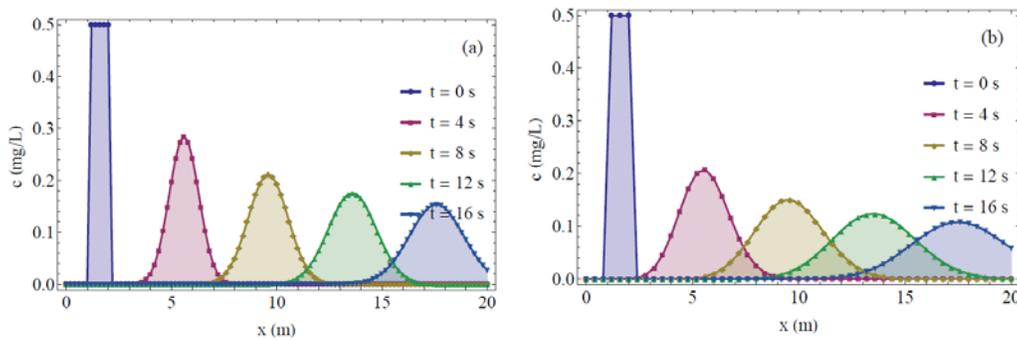


Figure 4: Numerical solution of the advection equation ($v = 1$ m/s; $R = 1$; $\lambda = 0$ s⁻¹) using the Finite Differences (a) using $C_r = 0.5$, and (b) $C_r = 0.25$.

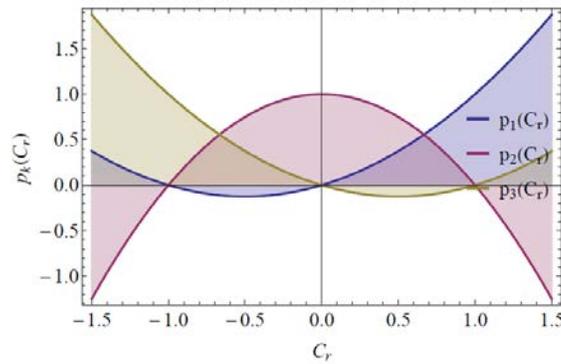


Figure 5: Polynomials $p_k(C_r)$ of Lax-Wendroff Method

For a Courant number $C_r = 1$, the Lax-Wendroff polynomials correspond to $p_1=1, p_2=p_3=0$. In this case, the exact analytical solution, $c_k^{n+1} = c_{k-1}^n$, is obtained as was also the case when using Finite Differences. However, numerical dissipation is also observed when using the Lax-Wendroff method if values of $C_r < 1$ are assumed. This is illustrated in Fig. 6(a), which shows the solution for the previous problem, involving a constant wave initial condition represented by Eq. (14), at different times ($t = 0, 4, 8, 12, 16$ s). The solution was obtained using Eq. (17) with $C_r = 0.5$.

An erroneous dissipation trend is also obtained when using the Lax-Wendroff method, although it appears less pronounced than that computed when using the Finite Differences method. On the other hand, a different type of numerical perturbation is observed in the Lax-Wendroff solution, which results in erroneous oscillations preceding the peak values. As the solution propagates in time, the peaks in the solution are observed to decrease while the oscillations are observed to increase with increasing x .

Fig. 6(b) illustrates the effect of the Courant number in predictions obtained using the Lax-Wendroff numerical approach. The solution is shown for the same times ($t = 0, 4, 8, 12, 16$ s) as those in Fig. 6(a), but using the Lax-Wendroff scheme (Eq. (17)) with $C_r = 0.25$. Dissipation also occurs in this case, but results show decreasing peaks for decreasing values of the Courant number. However, these lower peaks seems to be “compensated” with larger oscillations

preceding the peaks. The solution also lags behind for increasing time, with this effect being more pronounced for smaller values of C_r .

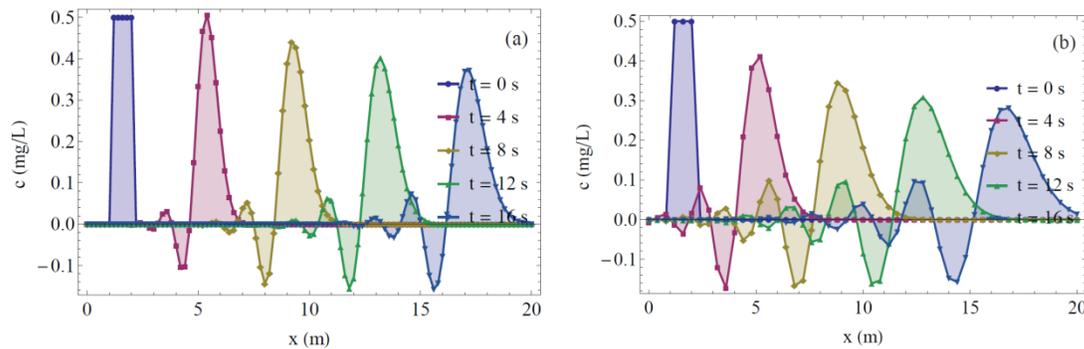


Figure 6: Numerical solution of the advection equation ($v = 1$ m/s; $R = 1$; $\Gamma = 0$ s) using Lax-Wendroff method, (a) using $C_r = 0.5$, and (b) using $C_r = 0.25$.

NUMERICAL SOLUTIONS OF ADVECTION PROBLEMS USING CIP METHOD

The cubic interpolated pseudo-particle method, CIP, proposed by Takewaki et al. (1985) and Takewaki & Yabe (1987), is used here to find an approximate solution $c(x, t)$ to advection problems that are also characterized by sorption and decay.

Although the CIP method has been previously used to solve hyperbolic equations (Yabe & Aoki, 1981; Kikuchi, et al., 2007), use of the CIP is developed in this study to solve the advective contaminant transport with linear sorption and first order decay, i.e., the advection-sorption-decay equation. The numerical evaluations presented in this paper were implemented in Mathematica codes.

For a given constant advection velocity $v_p > 0$, the solution should propagate the initial condition, displacing the solution by an amount equal to $\Delta x = v_p \cdot \Delta t$ during the time interval Δt . For this to happen, the following condition is adopted:

$$c(x, t) \cong c(x - \Delta x, t - \Delta t) \tag{21}$$

This condition is also illustrated in Fig. 7(a). In the CIP method (Yabe & Aoki, 1991), the discrete solution c_k^n at time n for a mesh of nodes x_k in the space domain x is smoothed by approximating a Hermite cubic polynomial $C(x)$ in the interval Δx between successive points $[x_{k-1}, x_k]$. The general form of the polynomial is given by:

$$C(x) = a_{k-1}^n \cdot (x - x_{k-1}^n)^3 + b_{k-1}^n \cdot (x - x_{k-1}^n)^2 + d_{k-1}^n \cdot (x - x_{k-1}^n) + e_{k-1}^n \tag{22}$$

The space derivative of the cubic Hermite polynomial is given by:

$$C'(x) = 3 \cdot a_{k-1}^n \cdot (x - x_{k-1}^n)^2 + 2 \cdot b_{k-1}^n \cdot (x - x_{k-1}^n) + d_{k-1}^n \tag{23}$$

The CIP method forces the polynomial approximation and its derivatives, $C(x)$ and $C'(x)$, to match the discrete values, $c(x, t)$ and $c'(x, t)$, at the extremes of each space interval $[x_{k-1}, x_k]$ (Fig. 7b):

$$c(x_{k-1}, t_n) = C(x_{k-1}^n) = c_{k-1}^n \quad \text{and} \quad c'(x_{k-1}, t_n) = C'(x_{k-1}^n) = c_{k-1}'^n \quad (24)$$

$$c(x_k, t_n) = C(x_k^n) = c_k^n \quad \text{and} \quad c'(x_k, t_n) = C'(x_k^n) = c_k'^n \quad (25)$$

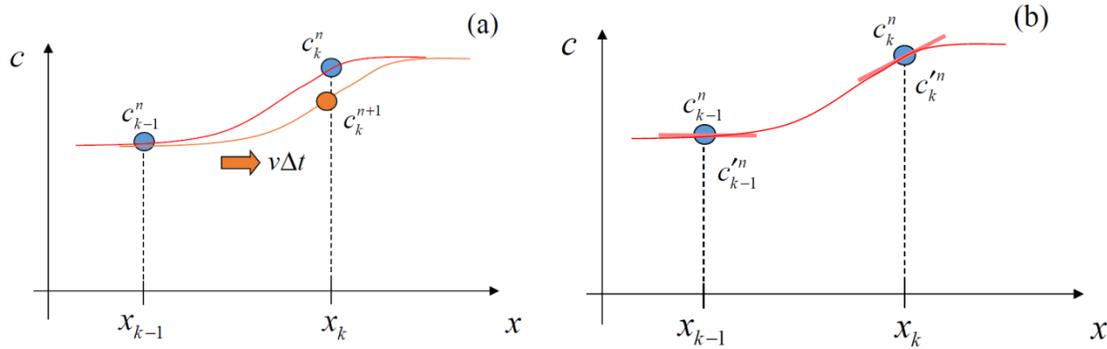


Figure 7: Hypothesis of CIP Method: (a) for the function $C(x)$ and, (b) for the function $C'(x)$.

Considering the approximation presented in Eq. (24) and using Eqs. (22) and (23), the coefficients d_{k-1}^n and e_{k-1}^n can be determined as:

$$d_{k-1}^n = c_{k-1}'^n \quad \text{and} \quad e_{k-1}^n = c_{k-1}^n \quad (26)$$

Noticing that $\Delta x = x_k^n - x_{k-1}^n = v_p \Delta t$ and applying the approximation presented in Eq. (25) to the nodes values in Eqs. (22) and (23), it is possible to determine the other coefficients a_{k-1}^n and b_{k-1}^n as:

$$a_{k-1}^n = \frac{(c_{k-1}'^n + c_k'^n)}{\Delta x^2} + \frac{2(c_{k-1}^n - c_k^n)}{\Delta x^3} \quad (27)$$

$$b_{k-1}^n = \frac{3(c_k^n - c_{k-1}^n)}{\Delta x^2} - \frac{(2c_{k-1}'^n + c_k'^n)}{\Delta x} \quad (28)$$

After having determined all coefficients, the discrete values of $c(x, t)$ and $c'(x, t)$ may be propagated to the next time step $n + 1$, as follows:

$$c_k^{n+1} = a_{k-1}^n \cdot (v_p \Delta t)^3 + b_{k-1}^n \cdot (v_p \Delta t)^2 + c_{k-1}'^n \cdot (v_p \Delta t) + c_{k-1}^n \quad (29)$$

$$c_k'^{n+1} = 3 \cdot a_{k-1}^n \cdot (v_p \Delta t)^2 + 2 \cdot b_{k-1}^n \cdot (v_p \Delta t) + c_{k-1}'^n \quad (30)$$

The CIP method should be used at time step n for all nodes in the space domain. This allows explicit determinations of c and c' for the next time step $n+1$. In this way, the initial solution at $t = 0$ h is propagated in time for as many time steps as necessary. It should be noted that the CIP scheme requires not only the values of the polynomial function in all nodes as an initial condition, c_k^0 , but also the values of the derivatives, $c_k'^0$. If these derivatives are not explicitly defined by a

continuous function, $c'(x, 0) = f'(x)$, it is still possible to estimate them using the central finite differences of the initial discrete function values, as follows (Moriguchi, 2005):

$$c_k^m = \frac{c_{k+1}^n - c_{k-1}^n}{2\Delta x} \quad (31)$$

The CIP method is expected to eliminate the dissipation and oscillation numerical problems observed when solving the advection equation using the Finite Differences and Lax-Wendroff methods with Courant numbers less than a unit. This is fundamental in order to achieve an efficient discretization of the problem both in the time and space domains.

The solution for the advection problem with the initial conditions defined by Eq. (14), was obtained using the CIP method and a Courant number $C_r = 0.5$. The predicted results are shown in Fig. (8) for different times ($t = 0, 4, 8, 12, 16$ s).

As shown in the Fig. (8), the predicted results are propagated in time without loss of information, dissipation or oscillations. The predicted results are considered to match well the analytical solution shown in Fig. 2(a). Also, the results in Fig. 8 illustrate clear superiority of the CIP method in relation to the predictions obtained using classical numerical techniques such as the Finite Differences method (Fig. 4) and the Lax-Wendroff method (Fig. 6).

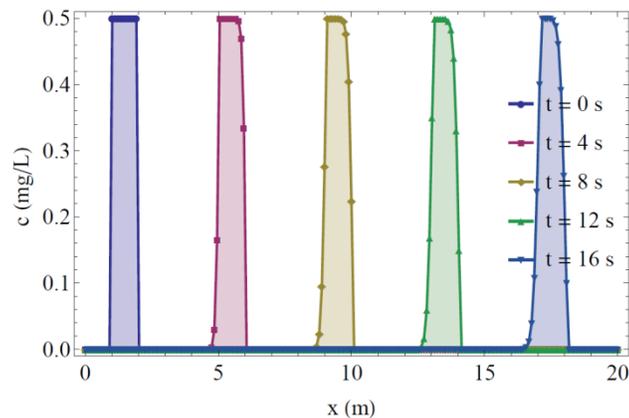


Figure 8: Numerical solution of the advection equation ($v = 1$ m/s; $R = 1$; $\lambda = 0$ s⁻¹) using the CIP method and Courant number $C_r = 0.5$.

NUMERICAL SOLUTIONS USING TRADITIONAL METHODS FOR ADVECTION PROBLEMS WITH LINEAR SORPTION ISOTHERM AND FIRST ORDER DECAY

Advection problems with linear sorption and first order decay have been conventionally solved numerically using Finite Differences by adopting a forward scheme in time and a backward difference in space. This approach leads to the following fully explicit algorithm (Xiao, 1996; Zienkiewicz & Morgan, 2006):

$$c_k^{n+1} = \left(1 - \frac{C_r}{R} - \lambda \cdot \Delta t\right) \cdot c_k^n + \frac{C_r}{R} \cdot c_{k-1}^n \quad (32)$$

Fig. 9(a) and 9(b) show the numerical solution of this problem obtained using Finite Differences and a Courant number of 0.5. The parameters used in these examples are the same as those used to obtain the exact solution presented in Fig. 2(c), 2(d) and 3(c), 3(d). That is, values $R = 1$ or 2 and $\lambda = 0.1 \text{ s}^{-1}$ were adopted.

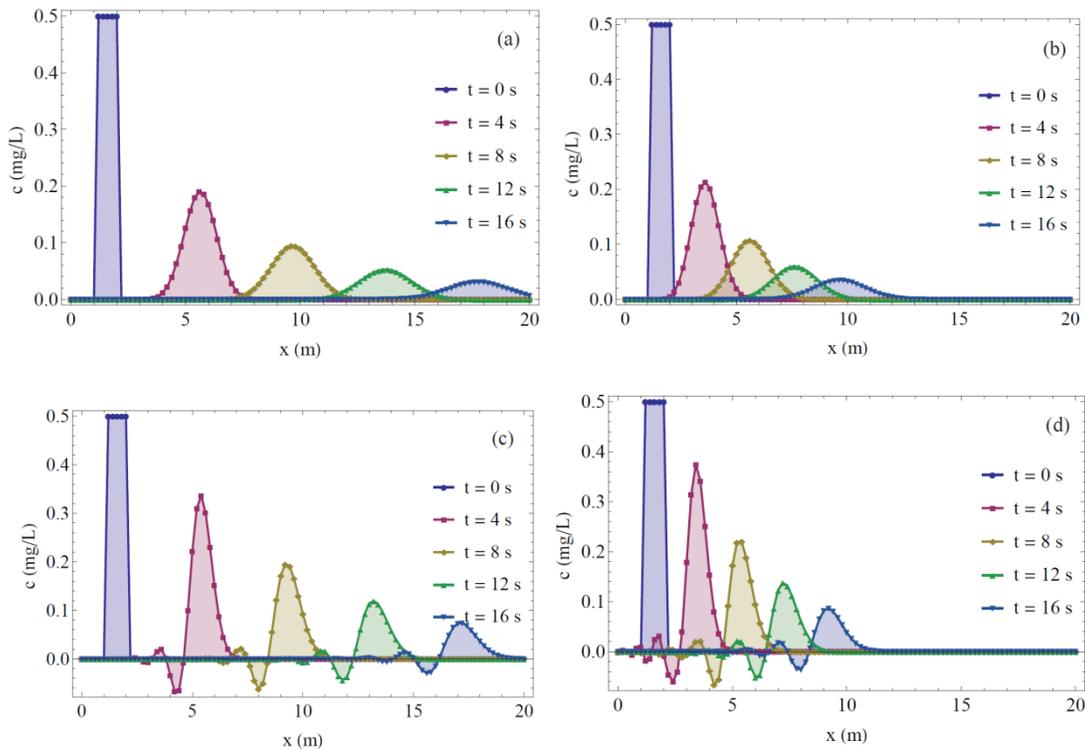


Figure 9: Numerical solution of the advection-sorption-decay equation with $C_r = 0.5$, obtained using: (a) Finite Differences without sorption nor decay ($v = 1 \text{ m/s}$; $R = 1$; $\lambda = 0.1 \text{ s}^{-1}$), (b) Finite Differences sorption and decay ($v = 1 \text{ m/s}$; $R = 2$; $\lambda = 0.1 \text{ s}^{-1}$), (c) Lax-Wendroff method without sorption nor decay ($v = 1 \text{ m/s}$; $R = 1$; $\lambda = 0.1 \text{ s}^{-1}$) and (d) Lax-Wendroff method with sorption and decay ($v = 1 \text{ m/s}$; $R = 2$; $\lambda = 0.1 \text{ s}^{-1}$).

In this case, the validity of numerical solutions may be particularly difficult to assess even when the general trend of the exact solution is known. This is because of the difficulty to establish whether the dissipation trend observed in Fig. 9(a) and 9(b) are the product of actual physical phenomenon (e.g., sorption, decay processes), or they are due to numerical errors.

The approach proposed by Lax & Wendroff (1960) was modified in this paper in order to be also used to solve this problem. In this case, the following fully explicit algorithm can be deduced to be applied to the advective phenomenon with linear sorption and first order decay:

$$c_k^{n+1} = p_4(C_r, R, \lambda) \cdot c_{k-1}^n + p_5(C_r, R, \lambda) \cdot c_k^n + p_6(C_r, R, \lambda) \cdot c_{k+1}^n \quad (33)$$

with,

$$p_4(C_r, R, \lambda) = \frac{C_r}{2R} \left[(1 - \lambda \Delta t) + \frac{C_r}{R} \right] \quad (34)$$

$$p_5(C_r, R, \lambda) = \left[1 - \lambda \Delta t + \frac{\lambda^2 \Delta t^2}{2} - \frac{C_r^2}{R^2} \right] \quad (35)$$

$$p_6(C_r, R, \lambda) = \frac{C_r}{2R} \left[\frac{C_r}{R} - (1 - \lambda \Delta t) \right] \quad (36)$$

When $R = 1$ and $\lambda = 0 \text{ s}^{-1}$, Eqs. (32) and (33) reduce to the advection case presented in Eqs. (15) and (17). Fig. 9(c) and 9(d) present the results obtained using the Lax-Wendroff method after adopting the same parameters used to define the exact solution shown in Fig. 2(c), 2(d) and 3(c), 3(d), (i.e., $R = 1$ or 2 , $\lambda = 0.1 \text{ s}^{-1}$).

NUMERICAL SOLUTIONS USING CIP METHOD FOR ADVECTION PROBLEMS WITH LINEAR SORPTION ISOTHERM AND FIRST ORDER DECAY

The CIP method was found to efficiently solve advection problems such as that represented by Eq. (1). This problem corresponds to hyperbolic equations for which dissipation phenomena are not present or may be considered negligible. In order to use the CIP method to simulate the transport model represented by Eq. (11), the problem should be solved by considering two components: an advective (Lagrangian) component, and a non-advective (Eulerian) component.

Accordingly, Eq. (11) which governs advection with sorption and decay processes was divided into non-advective and advective components. The equation governing the non-advective process is as follows:

$$c_t = -\lambda \cdot c \quad (37)$$

while the equation governing the advective process is as follows:

$$c_t + \frac{v_p}{R} \cdot c_x = 0 \quad (38)$$

The CIP method should be applied to the advective equations, thus avoiding the introduction of spurious numerical dissipations in the solution that result when using traditional numerical schemes. The non-advective equations may still be solved using classical methods such as the Finite Differences Method (FDM). In this case the Finite Differences scheme for the non-advective component, Eq. (37), can be written as:

$$\bar{c}_k^{n+1} = (1 - \lambda \cdot \Delta t) \cdot c_k^n \quad (39)$$

The analytical solution for this one-dimensional first order decay equation is given by:

$$c(x, t) = c_0 \cdot \exp(-\lambda \cdot t) \quad (40)$$

Fig. 10(a) and 10(b) show the results obtained for the non-advective equation (Eq. (37)) using the FDM ($C_r = 0.5$) and the exact analytical solution (Eq.(40)), respectively. The numerical prediction shows a very good agreement with the analytical results. In fact, errors were found to be less than 0.1%.

After solving the non-advective component (Eq. (37)), at a given time $n+1$, the solution \bar{c}_k^{n+1} , obtained from Eq. (39), is used as the initial condition c_k^0 in the CIP method to solve the advective component. The derivative $c'_k{}^0$ is obtained using Eq. (31).

The CIP method was used to find the solution of Eq. (11) after $n+1$ time steps. Fig. 11 presents the results obtained using the CIP method. The parameters adopted in this problem are the same as those used in the exact solution presented in Fig. 2(c), 2(d) and 3(c), 3(d) (i.e., $R = 1$ and 2 , $\lambda = 0.1 \text{ s}^{-1}$). Values of $C_r = 0.5$ were used in the predictions. As shown in Fig. 11, the numerical prediction matches very well the analytical solution presented in Fig. 2(c) and 2(d). No decay or oscillations due to numerical errors appear in the results using the CIP method. The good quality of these predictions is in clear contrast with that of the predictions shown in Fig. 9, which had been obtained using the FDM and Lax Wendroff Methods (Fig. 9).

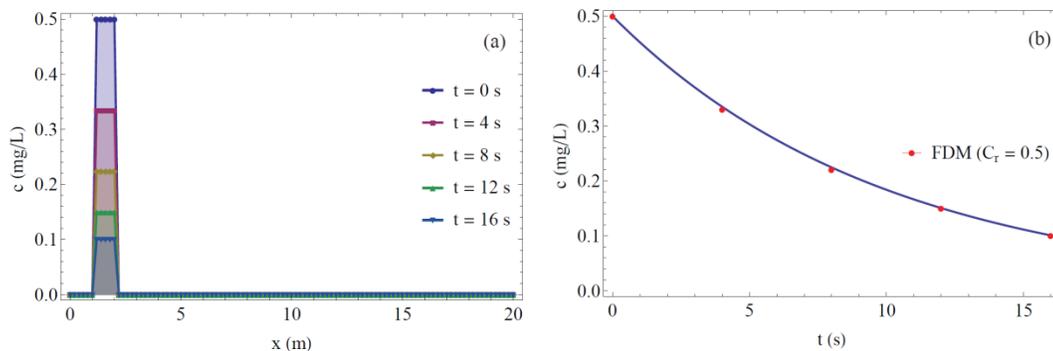


Figure 10: Numerical solution of the non-advective component (decay $\lambda = 0.1 \text{ s}^{-1}$): (a) obtained using FDM, with $C_r = 0.5$ and, (b) Analytical solution.

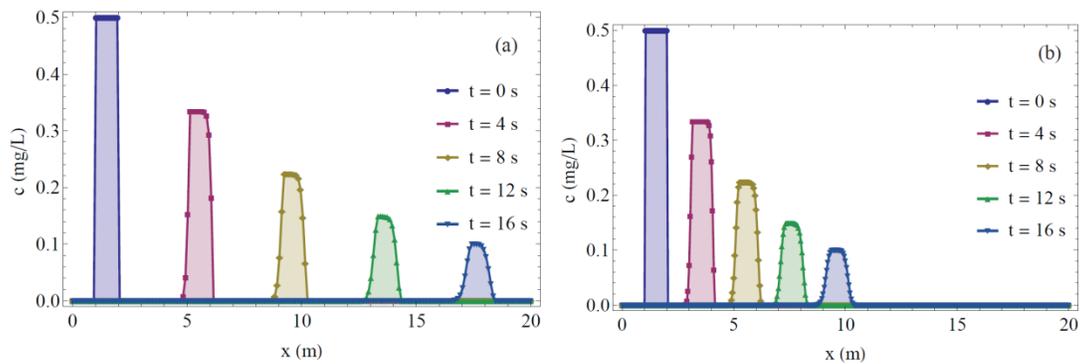


Figure 11: Numerical solution of the advection-sorption-decay equation with $C_r = 0.5$, using the CIP Method: (a) without sorption nor decay ($v = 1$ m/s; $R = 1$; $\lambda = 0.1$ s $^{-1}$), (b) with sorption and decay ($v = 1$ m/s; $R = 2$; $\lambda = 0.1$ s $^{-1}$).

As discussed in the paper, the non-advective component of the transport process is solved using the finite difference method. However, it should be noted that if this non-advective component meets the numerical stability criteria, the CIP method presented in this work can be easily extended for use in any other linear partial differential equations with an advective component. This includes a dispersion component in Eq. (2), which would allow using the CIP method to model the transport of contaminants that consider processes other than those considered in this paper.

CONCLUSIONS

This paper introduces a new numerical scheme, the Cubic Interpolated Pseudo-particle (CIP) method, to solve the hyperbolic differential equation that represents advection problems involving linear sorption and first order decay processes. The method is used to provide numerical solutions to problems involving advective, sorption and decay mechanisms, ultimately resulting in a new, superior numerical approach to this problem. The benefits of the new scheme is evaluated by comparing the numerical predictions against known analytical solutions and other common numerical schemes, including: (a) the explicit Finite Differences Method with forward derivatives in time and backwards derivatives in space; and (b) the Lax-Wendroff method. The various numerical solutions were compared to the exact analytical solution of transport problems characterized by having a constant wave as the initial condition.

The solution obtained using Finite Differences was found to be conditionally stable but to present spurious numerical dissipation errors for schemes involving Courant number smaller than one. This undesirable dissipation effect led to increasing dumping of the solution for decreasing Courant numbers. Therefore, the solution was found to rapidly deteriorate when using small time intervals.

The solution obtained using the Lax-Wendroff method was found to provide a slightly better approximation than that provided by the Finite Differences method. However, this method was found to also produce spurious numerical effects. They included solutions with erroneous oscillations and retardations. These undesirable effects were found to be more pronounced for smaller Courant numbers.

Ultimately, only when selecting the value of Courant number $C_r = 1$, the Finite Differences and Lax-Wendroff methods were found to produce results that compare well with the exact solution. However, selection of this value of C_r results in interdependent time and space discretizations. Such an ideal discretization can only be achieved in simple one-dimensional problems with equal intervals in the space domain.

The CIP method was found to successfully overcome the numerical problems observed when using the other two numerical schemes. Specifically, the initial constant wave was found to propagate in time and space without undue dissipations or oscillations. The good match of the numerical solution against analytical results was found to be independent of the adopted Courant number. Consequently, this method was found to allow highly efficient and independent discretizations in time and space.

Overall, the CIP method shows significant potential for applications in environmental problems. This is because many problems have at least one component in their governing equations that corresponds to advective mechanisms. In these cases, the results of this study show that the governing equations can be solved using the CIP method without introducing spurious numerical effects.

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