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# Numerical simulation of the advection-diffusion-reaction equation using finite difference and operator splitting methods: Application on the 1D transport problem of contaminant in saturated porous media

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**Abstract.** The combined advection-diffusion-reaction (ADR) equation, which describe the transport problem of a contaminant in porous medium, does not generally admit an analytical solution. In general, when solving the ADR equation, the numerical methods (such as finite differences, finite elements, splitting), for most practical problems, the ADR equation is too difficult to solve analytically. The finite difference method is the oldest and most commonly used method for the numerical solution of this kind of equation. Although newer techniques, such as those based on finite elements and splitting are appropriate for the solution of equilibrium-type problems, the finite difference remains the most appropriate for the solution of time-dependent phenomena. The transport of a contaminant can also be written by the ADR equation; hence, our objective is to choose the most efficient method to study the 1D transport problem of a contaminant and its evolution in a porous medium. In this work, we will simulate the ADR equation using two different methods: those of finite difference and splitting ones. The numerical result will be compared with the analytical solution in order to discuss the stability and the convergence of each of them using those two different methods. In the end, we will show that the splitting technical method is more efficient for solving this kind of problems in comparison with the finite difference method despite the fact that the latter is the most widely used by researchers. The validation of the efficiency of this method, implemented in this simulation, is tested on a 1D-transport problem of contaminant in a saturated porous medium.

## 1 Introduction

Partial differential equations have attracted increasing attention because they have applications in various fields of science and engineering. They can describe many physical, chemical processes and biological systems [1], [4], [6], [9], [8], [11]. As example advection-diffusion-reaction equations.

The combination of the advection, diffusion and reaction equations describes physical phenomena, matter or other physical quantities that are transferred into a physical system because of these three processes: advection, diffusion and reaction.

This combination is named, advection-diffusion-reaction equation, and can be written in the following form [2]:

$$\frac{\partial C}{\partial t} - V * \frac{\partial C}{\partial x} + D * \frac{\partial^2 C}{\partial x^2} - \lambda * C = 0 \quad (1)$$

With:

C: concentration of the mass transfer species.

D: The diffusivity constant for mass.

V: the component of the velocity of the carrier fluid

λ: The decomposition rate.

In general, these equations do not admit any analytical solution except in very simplified cases. This is why a recourse to numerical solving methods is necessary. These methods can be applied in several fields, notably in chemistry, environmental sciences, hydrology, geology, petroleum engineering and biology, etc. [1], [4], [6], [9], [8], [11][13].

The most commonly used methods for the numerical solution of this type of equation is the finite difference as mentioned above [6], [11], [9]-[8]. As there is also the splitting method, also called the operator splitting method, which is a powerful method for the numerical study of complex models [2], [9], [11]. The idea of operator splitting methods based on dividing a complex problem

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into a sequence of simpler tasks, called splitting sub-problems.

In this paper, we will introduce two different methods of dividing advection-diffusion-reaction equations. Those of the finite difference approach, which is a common technique for solving partial differential equations with an approximate solution. It consists in solving a system of relations (numerical scheme) linking the values of unknown functions at certain points sufficiently close to each other [3]. And the Splitting method, which is a method that replaces a single scheme to solve a complicated PDE (Partial differential equation) with a sequence of simpler schemes that solve the linked PDEs and solve together the original PDE (Partial differential equation) (up to a specified order of precision). Finally, we will compare between these two methods in terms of stability and convergence.

This document is organized as follows. In the next section, we will discuss the splitting, and finite difference methods used to solve our ADR equation. The third section will tackle the numerical result of our example. We will afterwards compare between the exact and numerical solution.

# 2 METHODOLOGY

In this work, we will focus on two different methods of mathematical representation, that of splitting and that of the finite difference, discussing the stability of each method and spotting the most efficient of them in the following sections.

## 1.1 Mathematical description of the problem

As indicated in section 1, the problem to be solved is that of the numerical study of the advection-diffusion-reaction problem, with two different techniques namely, finite difference and splitting methods. Which can be written in the following form, as mentioned above:

$$\frac{\partial C}{\partial t} - V * \frac{\partial C}{\partial x} + D * \frac{\partial^2 C}{\partial x^2} - \lambda * C = 0$$

Where C is the concentration of the mass transfer species, D is the diffusivity constant for mass; V is the component of the velocity, λ and is the decomposition rate, noting the temporal and spatial step sizes by Δt and Δx, respectively.

## 1.2 Numerical method

### *1.2.1 The finite difference method*

We discretize the advection-diffusion-reaction equation using a first-order forward difference for the time derivative, and a symmetric (second-order) difference for the space derivative, and the equation can be written as: [1].

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} - V * \frac{U_i^n - U_{i-1}^n}{\Delta x} + D * \frac{U_{i+1}^n - 2 * U_i^n + U_{i-1}^n}{\Delta x^2} - \lambda * U_i^n \quad (2)$$

Noting that the equation is stable for Cr≤1 and R≤1/2 and $\Delta t \leq \frac{\Delta x^2}{V*\Delta x + 2*D}$. [8]The number of Current Cr for advection is calculated as V*Δt/Δx, and the stability for diffusion R is calculated as D*Δt/Δx2.

### *1.2.2 The splitting method*

Using operator splitting method, our ADR equation will be divided into two sub-problems, which will be treated by the finite difference method. This mean that each part will be treated individually[14], [26]. The principle of this method is that, the first equation (advection) will be solved for a time interval of Δt using the initial condition of the principal equation (equation 1). The result obtained from there will be the initial condition of the second equation (diffusion-reaction). This equation will be solved for a time interval of Δt and the solution of principal equation (equation 1) will be obtained for a time interval Δt. In the end, the problems will be solved consecutively by combining them with the initial conditions.

Using the previous finite difference schemes, the corresponding division scheme for solving the 1D advection-diffusion-reaction equation by the Splitting method is [4], [5], [6]:

$$\frac{\partial C_1}{\partial t} + V * \frac{\partial C_1}{\partial x} = 0 \quad C_1(t_n, x) = C(t_n, x) \in [t_n, t_{n+1}] \qquad (3)$$

$$\frac{\partial C_2}{\partial t} = D_x \frac{\partial^2 C_2}{\partial x^2} - \lambda * C_2 \qquad C_2(t_n, x) = C_1(t_{n+1}, x) \in [t_n, t_{n+1}] \qquad (4)$$

Noting that the equation is stable for Cr≤1 and R≤1/2 and $\Delta t_{AD} \leq \min(\Delta t_A, \Delta t_D)$ [1]–[5]

With: [1]

$\Delta t_A \leq \frac{\Delta x}{V}$ : The time step for advection equation.

$\Delta t_D = \frac{\Delta x^2}{2*D}$ : The time step for diffusion-reaction equation.

As already mentioned, our sub-problem will be treated by the finite difference method, where our algorithm becomes as follows:

$$C_{1_i} = C_i - \frac{V*\Delta t}{\Delta x} * (C_i - C_{i-1}) \qquad (5)$$

$$C_{2_i} = C_{1_i} + \frac{D * \Delta t}{\Delta x} * (C_{1_{i+1}} - 2C_{1_i} + C_{1_{i-1}}) - \lambda * C_{1_i} \qquad (6)$$

## 3 APPLICATION

In this part, a one-dimensional advection-diffusion-reaction equation will be solved with the operator splitting method and the finite difference one. The result will be examined for different value of λ (the decomposition rate). Then it will be compared to the exact solution. In addition, the accuracy of the methods will be evaluated by calculating error standards. This kind of error is calculated as follows [4]:

$$Error = \Delta x * \sqrt{sum(C^{exact} - C^{Numerical})^2}$$

In our case, the data are as follows [4], [15]:

**Table 1.** The data of example

| | |
|---|---|
| The exact solution | $C^{exact} = \frac{\exp^{-\lambda * t}}{\gamma} * \exp^{-(\frac{x - x_0 - V*t}{L*\gamma})^2}$ With: $\gamma = \sqrt{1 + \frac{4*D_x*t}{L^2}}$ |
| The initial condition | $C(x,0) = \exp^{-(\frac{x-x_0}{L})^2}$, $x_0 = \frac{1}{4}$ |
| The boundary condition | $C(0,t) = C(L,t) = 0$ |
| The velocity | $V = \frac{C_r * \Delta x}{\Delta t}$ |
| The diffusion coefficient | $D_x = \frac{V * \Delta x}{2 * P_e}$ |
| The number of Current | Cr=1 |
| The Peclet number | Pe=100 |
| The spatial step | $\Delta x = 0.0005$ |
| The temporal step | $\Delta t = 0.005$ |
| length of the medium | as L = 1 |

Figures 1, 2, 3,4 and 5 show the result obtained using the operator splitting and the finite difference methods:

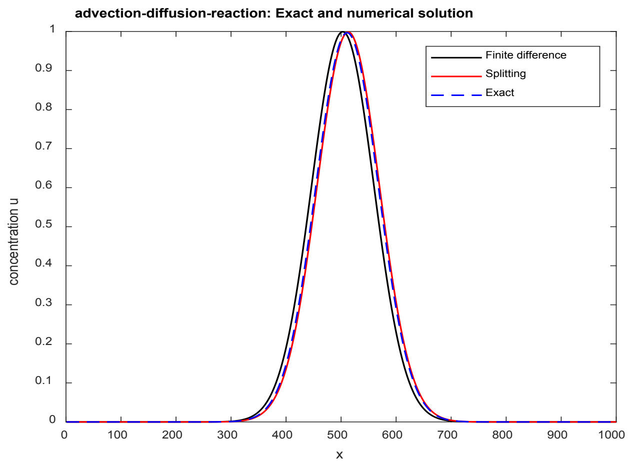


**Fig. 1.** ADR with Splitting and Finite difference methods with λ=0.001

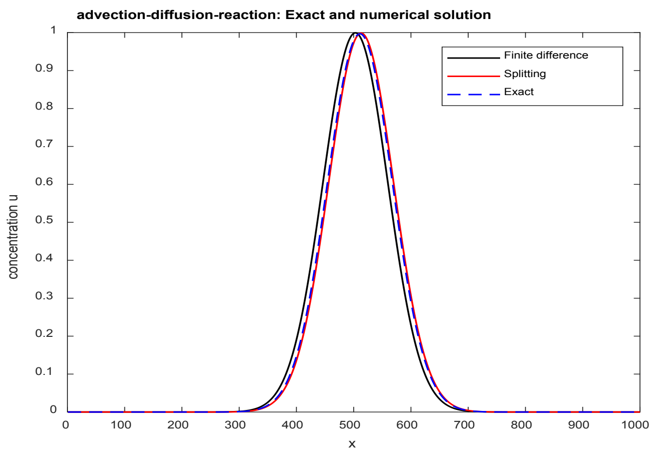


**Fig.2. ADR** with Splitting and Finite difference methods with λ=0.01

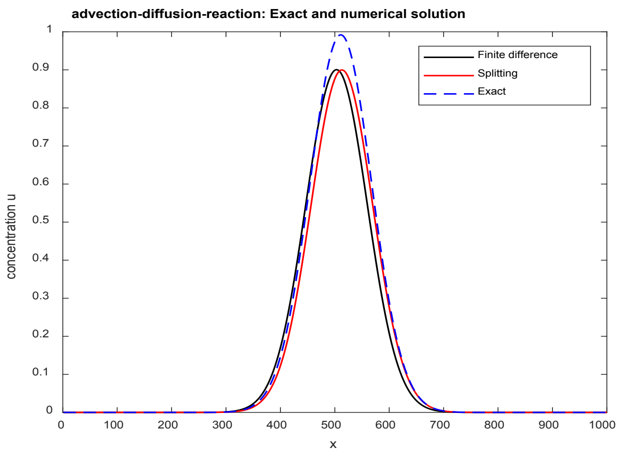


**Fig. 3.** ADR with Splitting and Finite difference methods with λ=0.1

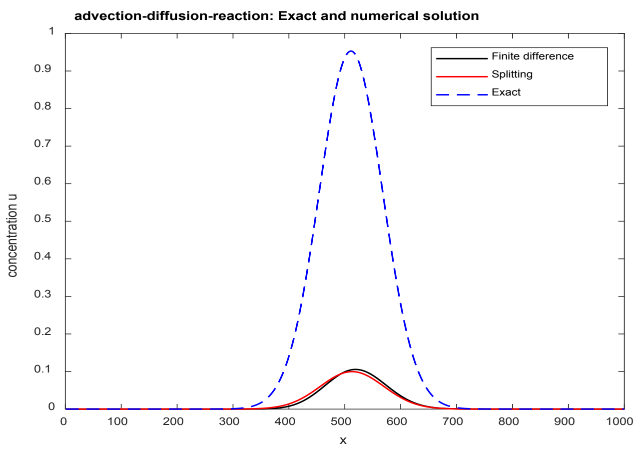


**Fig.4. ADR** with Splitting and Finite difference methods with λ=0.9

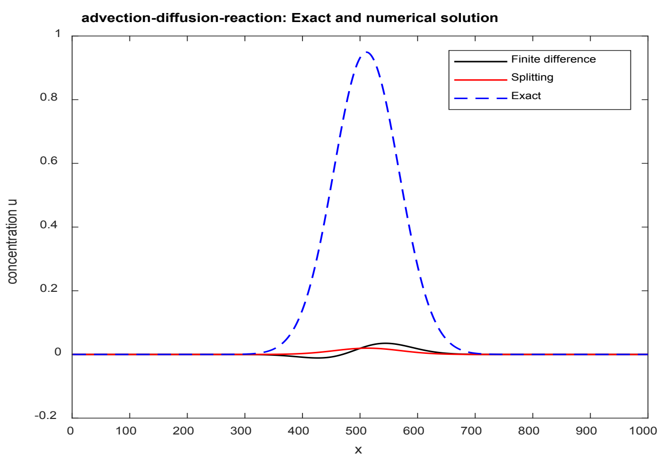


**Fig.5. ADR** with Splitting and Finite difference methods with λ=0.98

The calculations in Table 1 give the error value for the two different methods, with different values of λ:

**Table 2.** The Error value with different λ

| Error | Splitting | Finite difference |
|---|---|---|
| λ =0.0001 | $1{,}253.10^{-4}$ | $4{,}9\ .10^{-4}$ |
| λ =0,01 | $1{,}310.10^{-4}$ | $4{,}968.10^{-4}$ |
| λ =0.1 | $4{,}83.10^{-4}$ | $6{,}55.10^{-4}$ |
| λ =0.9 | 0.0043 | 0.0043 |
| λ =0.98 | 0.0046 | 0.0047 |

According to table 1, we notice that when the value of λ decreases, the error decreases, hence the numerical solution becomes closer to the exact solution. As we can also see, the splitting method is more efficient than the finite difference one.

## 4 EXAMPLE OF 1D CONTAMINANT TRANSPORT

In our work, we will deal with the case of the 1D transport of a contaminant within a soil-groundwater system, by changing the value of λ. To prove the results found before. The following is the exact solution to this problem: [14]

$$C_{exact} = exp^{\sqrt{(\frac{V}{2}*D)^2}} * erfc(\frac{x + \left(\sqrt{V^2 + 4 * \lambda * D}\right) * t}{\sqrt{4 * D * t}}$$

$$+ exp^{\frac{-\sqrt{\left(\frac{V}{2*D}\right)^2} * x}{2}}$$

$$* (erfc(\frac{x - \left(\sqrt{V^2 + 4 * \lambda * D}\right) * t}{\sqrt{D * D * t}}$$

With an initial, condition equal to:

$C(X, 0) = 0.$

In addition boundary condition equal to :

$C(0, t)$ =1 and $C(L, t) = 0.$

In our case, the velocity of the flow and diffusion coefficient is taken as:

V=0.1 and D=0.5 With $\Delta x = 0.1$ and $\Delta t = 0.01$, as well as the length of the medium is chosen and is given as L= 10

Hence, we will apply these two methods to our contaminant transport case, to confirm the efficiency of the Splitting method.

Fig 6, 7,8 and 9 show the result obtained using the operator Splitting method and finite difference method.

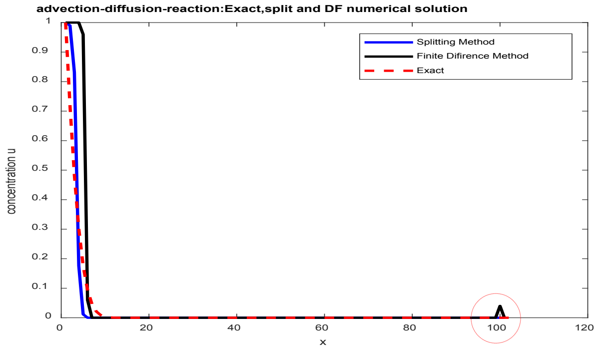


**Fig. 6.** ADR with Splitting and Finite difference methods with λ=0.000001

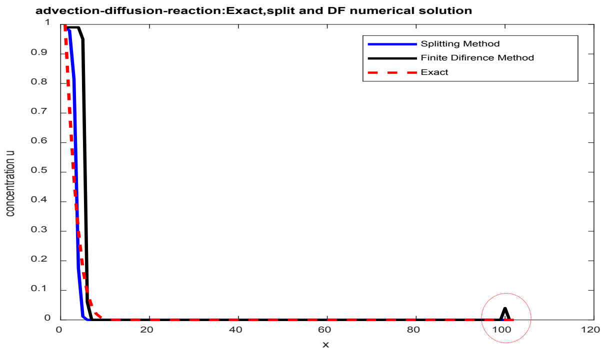


**Fig. 7.** ADR with Splitting and Finite difference methods with λ=0.01

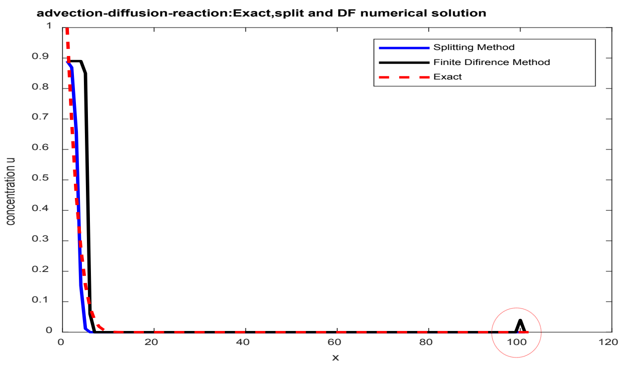


**Fig. 8.** ADR with Splitting and Finite difference methods with λ=0.11

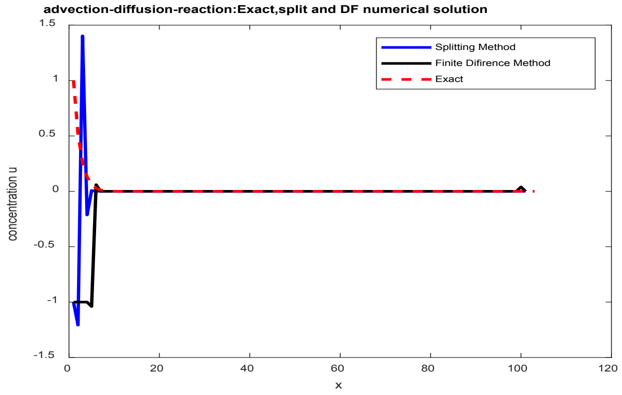


**Fig. 9.** ADR with Splitting and Finite difference methods with λ=2

**Table 3.** The Error value with different λ

| | Splitting Error | Finite difference Error |
|---|---|---|
| λ =0.00001 | 0.1231 | 0.13 |
| λ =0.01 | 0.1275 | 0.1395 |
| λ =0.11 | 0.1784 | 0.1837 |
| λ =2 | 0.2401 | 0.2977 |

According to the four figures and table 3 , it can be pointed out that the numerical solution approaches the exact solution for very small values of λ, for the two methods but we can notice it is not stable at one hundred percent for the small ones values for the finite difference method. However, there is an instability of the numerical solution for large values of λ for the finite difference method. On the other hand, there is an instability of the numerical solution for very large values of λ for the two methods.

## 5 CONCLUSION

This paper looks at two strategies for solving the advection-diffusion-reaction equation: the finite difference method and the Splitting method.

The purpose of this research is to compare their error values and determine the best effective methods for researching contaminant evolution.

We demonstrated that the inaccuracy of the two methods is quite modest for very small values of λ during the simulation. It was also discovered that as the value of λ grows larger, the numerical scheme obtained using the finite difference method becomes unstable. The numerical scheme derived using the Splitting technique, on the other hand, remains stable, if not more so, for small values of λ, but converges to the precise solution for extremely small values of λ. As can be seen, the numerical and precise solutions for the Splitting approach are in agreement.

As a result, we can conclude that this method outperforms the finite difference method. For that reason, the splitting method is more useful for numerically simulating this type of transport as well as studying the movement of a contaminant in any medium.

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