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# 1-D Numerical Simulation of Transport and Biodegradation in Saturated Porous Media

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**Abstract**

Biological restoration is a promising technique for the treatment of polluted sites. It consists in stimulating the activity of the bacteria which are present in an environment by the contribution of nutritive substrates such as oxygen and nitrogen.

In this work, we will focus on the mathematical and numerical modeling of the 1D problem of transport and biodegradation of a contaminant in a saturated porous medium because this type of problems is often encountered in saturated aquifers with pollution sources.

The mathematical model that we will formulate is a coupled system that takes into account the effect of advection, diffusion and biodegradation of the substrate in the medium. In this context, we are interested by the numerical simulation of this system in order to show the effect of biodegradation, as a remediation technique, on the transport of a contaminant.

The mathematical model under consideration is composed of three independent equations linked together, since each term must be treated with the appropriate numerical method. Additionally, in the literature we do not find any detailed study that present the numerical approach to follow so as to solve this type of systems. Making it difficult to solve numerically.

Therefore, our objective in this work is to develop a new strategy that will allow us to approach this type of problem and produce results that are more efficient.

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The technique used here is based on the operator splitting method, which is an effective method to solve this kind of complex models. The primary idea behind this strategy is to break down a complex problem into smaller subsystems, known as division sub-problems, and to solve each one of them using the proper numerical method.

The transport problem is approximated by a finite difference scheme, first order backward difference for the term of advection and a second order symmetric difference for diffusion term, and the biological equations, which are presented using Monod kinetics, are solved by a Rung-Kutter method of order 4.

Several numerical tests will be presented with and without biological restoration to show the importance of the biodegradation technique as a remediation procedure.

The operator splitting method employed in this simulation is validated using an example of transport and biodegradation with first order kinetics (case of low contaminant concentration) that admits an analytical solution in saturated porous media. The numerical and analytical results are in perfect agreement.

**Keywords**: Transport, Biodegradation, Saturated porous media, Finite different scheme, Splitting technique, Runge- Kutta method.

## I. INTRODUCTION

The problem of transport through a saturated porous media includes many processes such as advection, diffusion, and zero order or first order production and decay.

Transport problems are being widely encountered in many scientific and technical fields, and in recent years many theoretical analyses and extensive numerical simulations have been conducted to solve them [1]. For example, theoretical solutions have been derived for the problems of evolution of pollutants in the underground environment in which the process of transport of reactive solutes coupled to the flow of water within a saturated heterogeneous porous medium [2]. There are also many studies that have been done on the transport of the contaminant in porous media under biodegradation reaction [2]- [4-5].

In recent years, a number of researches have suggested the importance of biodegradation of contaminants in a porous media (ref). Therefore, transport and biodegradation modeling have attracted interest from various fields including medicine, biology, bioremediation, chemistry, water treatment and engineering [1]–[4]. This modeling is treated as a coupling of three different terms, advection, diffusion and biological terms [5], and each term requires a specific treatment to be solved numerically, hence it has become one of the most important problems in numerical simulation.

In this work, we are interested in the one-dimensional modeling of the problem of contaminant transport and biodegradation in a saturated medium because, the majority of the flows in the saturated aquifers are one-dimensional, and several texts were made in 1D [6-7]. Also, there are not enough numerical studies that focus on solving this type of problem. And since the majority of these problems admit an analytical solution, so we can validate our numerical approach that we will adapt by comparing the numerical results with the analytical ones [8].

Furthermore, many one-dimensional exact analytical solutions in closed form have been proposed, and the attention of scientists has been devoted to solutions with time-dependent sources [9]. A library of one-dimensional analytical models that encompasses some solutions with decaying sources has been proposed by Van Genuchten et al. [10]. Guerrero et al [11] proposed an approach based on Duhamel's theorem to compute one-dimensional solutions.

There are numerous analytical solutions to the 1D transport problem in the literature.

These analytical solutions can be used to generate pollution scenarios for risk analysis, investigate the influence of physico-chemical parameters on pollutant transport, and verify numerical models [10-12]. From where the choice of the 1D model.

In this context, our problem is not only the flow but we are also more interested in the coupled system that gathers a set of phenomena such as transport and biodegradation. And as already mentioned our goal is to develop a new technique that will enable us to handle this type of problem in a more efficient manner.

The mathematical model is a coupled system that includes advection and diffusion terms as well as a biodegradation term that is presented here by a Monod kinetic [6]-[8].

To deal with this coupled system, an operator splitting approach, also called the splitting method, is proposed to solve this system, which allows treating separately the different terms of the mathematical model [5].

The method separates the transport and reaction phases (biodegradation term). Therefore, a finite difference approach is used first to solve the transport problem, first order backward difference for the term of advection and a second order symmetric difference for diffusion one. The concentrations acquired at this stage are then used as initial concentrations in the solution of the reaction equations, which are represented as ordinary differential equations (ODEs) and solved using the Runge-Kutta method of order 4 [9]-[10].

## II. THE MATHEMATICAL MODEL

We are in the presence of the problem of the one-dimensional transport of a substrate of concentration C and a nutrient, which is the oxygen of concentration O in a saturated porous medium. The substrate also undergoes the phenomenon of biodegradation with the help of microorganisms of concentration B presented in the medium.

The equations which describe the transport and biodegradation model are as follows:

### A. Advection-diffusion and biodegradation of the substrate and oxygen:

$$R\frac{\partial(\theta C)}{\partial t} = \nabla(\theta D_C \nabla C - \theta v C) + R_1(C,O,B) \quad (1)$$

$$\frac{\partial(\theta O)}{\partial t} = \nabla(\theta D_O \nabla O - \theta v O) + R_2(C,O,B) \quad (2)$$

**B. Development of bacteria:**

$$\frac{\partial B}{\partial t} = R_3(C,O,B) \quad (3)$$

**C. Darcy's law:**

$$\vec{V} = -\frac{K}{\mu}(\nabla P - \beta)\vec{e_z} \quad (4)$$

Where:

C: the concentration of the contaminant, O the concentration of oxygen, B the concentration of the microorganism, $D_o$ and $D_c$ are the diffusivity constant for mass and $v$ the component of the velocity of the carrier fluid, R is the retardation factor due to adsorption, θ is the coefficient of porosity, P is the pressure,μ is the viscosity of the mixture,β is the fluid density, K is the permeability tensor of the porous medium.

$R_1$(C, O, B), $R_2$(C, O, B) and $R_3$(C, O, B) are the biological terms that describe biodegradation and are presented by the Monod model [15], which describes respectively the biodegradation of contaminant, oxygen, and organic microbes. We have therefore [15]:

$$R_1(C,O,B) = \frac{-\mu_0}{Y_C}B\left(\frac{C}{C+K_C}\right)\left(\frac{O}{O+K_O}\right) \quad (5)$$

$$R_2(C,O,B) = \frac{-\mu_0}{Y_O}B\left(\frac{C}{C+K_C}\right)\left(\frac{O}{O+K_O}\right) \quad (6)$$

$$R_3(C,O,B) = \mu_0 B\left(\frac{C}{C+K_C}\right)\left(\frac{O}{O+K_O}\right) - K_d B \quad (7)$$

With:

The term $\frac{\mu_0}{Y_C}$ defines the maximum oxygen utilization rate per unit mass of microorganisms and $Y_C$ is the mass of bacteria produced per unit mass of degraded contaminant [15].

The term $\frac{\mu_0}{Y_O}$ defines the maximum substrate utilization rate per unit mass of microorganisms and $Y_O$ is the mass of bacteria produced per unit mass of oxygen degraded [15].

The term $B\mu_0$ is positive and defines bacterial growth, where $\mu_0$ is given by Monod kinetics. The term $-K_dB$ is negative, and describes bacterial degradation, where $K_d$ defines the degradation constant. Kc is the half-saturation constant of the substrate and $K_O$ is the half-saturation constant of oxygen [15].

When the coefficient of porosity and the retardation factor due to adsorption flow remain constant in time and space (steady state flow) [9],[15]-[16], the system of equation reduces to :

$$\frac{\partial(C)}{\partial t} = \nabla(D_c \nabla C - vC) - \frac{\mu_0}{Y_C} B \left(\frac{C}{C+K_C}\right)\left(\frac{O}{O+K_O}\right) \tag{8}$$

$$\frac{\partial O}{\partial t} = \nabla(D_o \nabla C - vC) - \frac{\mu_0}{Y_C} B \left(\frac{C}{C+K_C}\right)\left(\frac{O}{O+K_O}\right) \tag{9}$$

$$\frac{\partial B}{\partial t} = \mu_0 B \left(\frac{C}{C+K_C}\right)\left(\frac{O}{O+K_O}\right) - K_d B \tag{10}$$

In the following section, we simulated the system (8)-(10) using the splitting method described above.

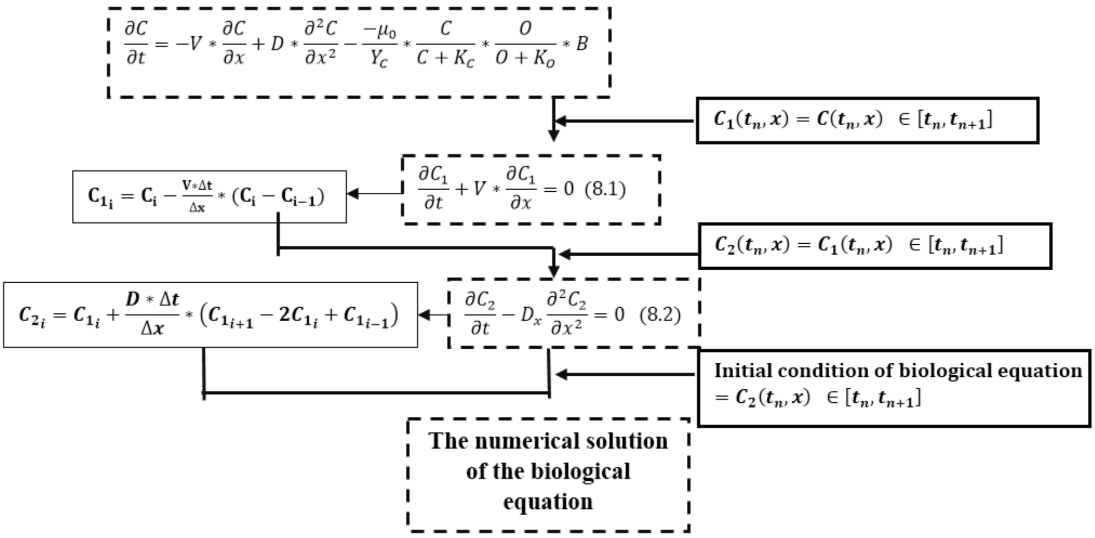
## III. NUMERICAL APPROACH

Our system of equations (8) and (9) will be divided in two sub-problems using the operator splitting approach, which will be solved using the finite difference method. This means that each problem will be solved by the appropriate method [5], [13]-[14].

The basic idea behind this method is that the first equation (advection) is solved for a time interval of Δt utilizing the main equation's initial condition. The result obtained from there will be the initial condition of the second equation (diffusion). This equation will be solved for a time interval of Δt.

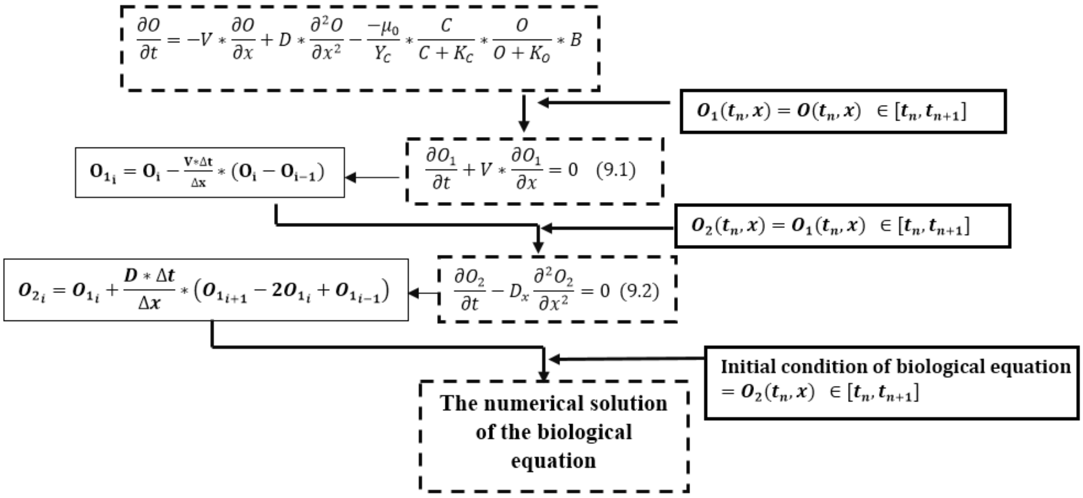
The finite difference approach will be used to discretize the advection and diffusion equations.

### A. Splitting the Substrate transport equation




In this case, the problem is divided into two sub-problems that of advection and diffusion where $C_1$ is the concentration in the advection process and $C_2$ is the concentration in the diffusion of the process. Equation (8), equation (8.1) and equation (8.2) represent the general equation, advection equation and the diffusion equation respectively. In the solution process, equation (8.1) will be solved for a time interval of Δt using the initial condition of equation (8). The result obtained from there will be the initial condition of equation (8.2). Then, equation (8.2) will be solved for a time interval of $\Delta t$. The result obtained from there will be the initial condition of biological equation. Thus, the problems will be solved consecutively by combining them with the initial conditions [12].

### B. Splitting the Oxygen transport equation




The problem is separated into two sub-problems in this case: advection and diffusion, with O1 representing the concentration in the advection process and O2 representing the concentration in the diffusion process. Equations (9), (9.1), and (9.2) represent the general equation, advection equation, and diffusion equation, respectively. The initial condition of equation (9) will be used to solve equation (9.1) for a time period of Δt in the solution process (9). The initial condition of equation will be the result acquired from there (9.2). Then, given a time period of Δt, equation (9.2) will be solved. The initial condition of the biological equation will be the outcome produced from there. Thus, the problems will be solved consecutively by combining them with the initial conditions [12].

The result obtained from there will be the initial condition of the biological equation, which will be solved using the Runge-Kutta method of the fourth order. Thus, the problems will be solved in order by combining them with the initial conditions.

## IV. NUMERICAL SIMULATION

In this section, we will study the numerical simulation of the one-dimensional transport of a contaminant that will be degraded by heterotrophic bacteria in a saturated porous medium.

We assume that these bacteria are immobile, but the oxygen and the substrate are moving along 'x' in this medium.

The biological and transport parameters used in the simulation are [11]:

> $V=1{,}0$ m.day$^{-1}$, $D_O=D_c=0{,}2m^2.day^{-1}$, $K_O= 0{,}1mg.L^{-1}$, $K_C=0{,}1mg.L^{-1}$, $K_d=1{,}0$ mg.L$^{-1}$, $Y_O=0{,}125$ L.mg$^{-1}$, $Y_C=0{,}125$ L.mg$^{-1}$, R=1, θ=0.4 $\mu_0=0{,}1$ mg.L$^{-1}$. With $\Delta x=0{,}2$m et $\Delta t=0{,}002$day.
>
> C(x,0)=10 mg/l and O(x,0)=9 mg/l.

Initially, no initial concentration of the bacteria is present in the medium. The initial distribution of substrate and oxygen concentration at time t = 10 days is shown in Figure1:

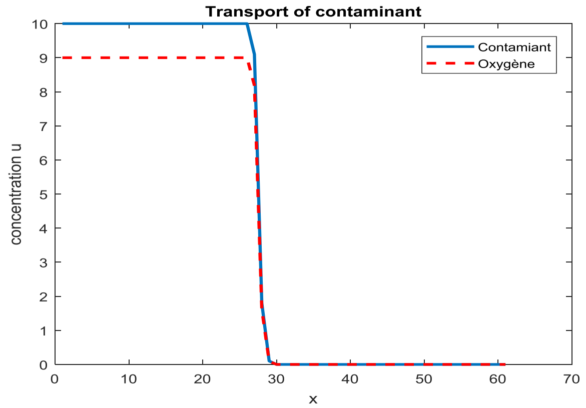



**Figure 1.** The profile of initial substrate and oxygen concentrations

The biological processes are then simulated by injecting 0.2 mg/l of heterotrophic bacteria. In figure 2, we show the profile of the concentrations of substrate, oxygen and bacteria after 10 days of bioremediation.

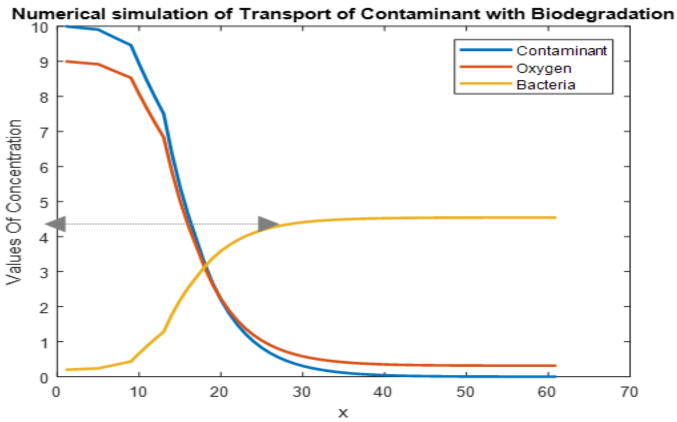



**Figure 2.** The profile of substrate concentrations after 10 days of bioremediation

In a second test, we simulate microbial activities in the medium. This time we inject 15 mg/l of oxygen from the entrance boundary of the domain. Figure 3 shows the substrate concentrations after 10 days of bioremediation and a significant increase in bacterial growth.

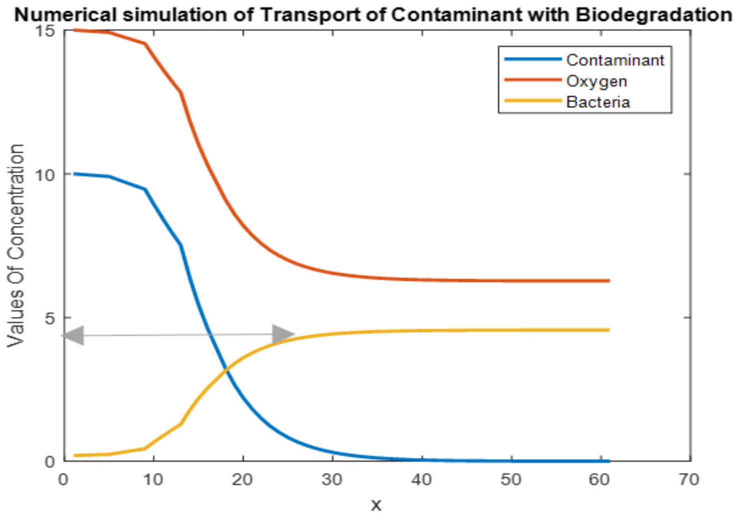



**Figure 3.** The profile of substrate concentrations after 10 days of bioremediation by injecting 15 mg of oxygen

Finally, the validation of the splitting technique used in this simulation was tested by comparison between numerical result and analytical solution for a one-dimensional problem of transport and biodegradation with a first order reaction (for small concentrations).

In our case the velocity of the flow and diffusion coefficient is taken as: $V=0{,}1cm.s^{-1}$, $D=2{,}5.10^{-7}cm^2.s^{-1}$, $\Delta x=0{,}0005cm$, $\Delta t=0{,}005s$

et $\lambda=0{,}0001\ s^{-1}$. [12] [24-25]

The exact solution to this problem is given as follows [12]:

$$C^{exact} = exp^{(-\frac{\lambda * t}{\gamma})} * exp^{(-\frac{(x-x0-V*t)^2}{\gamma})} \qquad (11)$$

Avec $\gamma = \sqrt{1 + \frac{4*D*t}{L^2}}$

With an initial condition equal to:

$$C(x,0) = exp^{(-\frac{(x-x0)^2}{L^2})} \qquad (12)$$

In addition, a boundary condition equal to:

$$C(0,t) = C(L,t) = 0$$

Figure 4, presented the analytical solution (exact solution) and the numerical solution obtained using the operator splitting method.

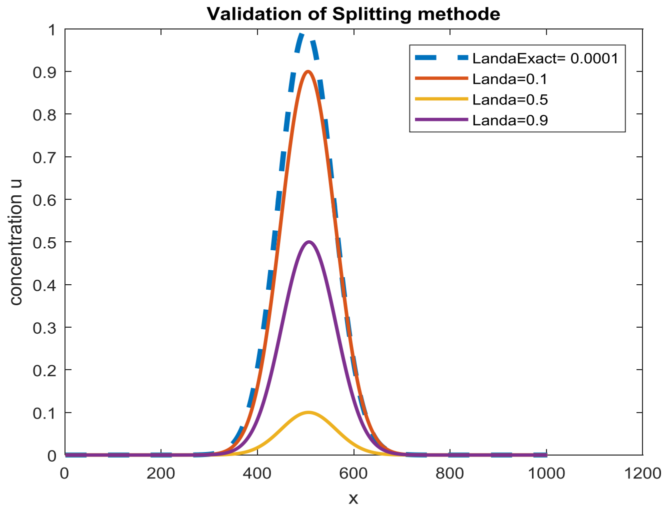



Figure 4 Analytical result in agreement with the numerical solution (blue curve) for one dimension with a first order reaction

According to figure 4, we can see that the numerical solution approaches the exact solution for any very small value of λ.

## CONCLUSION

In this work, we have developed a novel numerical approach able to solve a coupled system of transport and biodegradation in the one-dimensional case. This approach is based on the splitting technique. This procedure has the advantage of treating each subsystem that composes our mathematical model with the numerical method that adapted it. Thus, the advection and diffusion problem were treated by the finite difference method, which proved to be very efficient in the different tests presented.

The biological terms have been solved by the explicit Rung-Kutter method of order 4 with a time step chosen much smaller than that of transport.

The validity of the proposed numerical approach has been tested on a one-dimensional transport and biodegradation problem with first order degradation kinetics. The numerical solution is in good agreement with the analytical solution.

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