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Alternative approaches for groundwater pollution

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Abstract: This paper deals with the analysis of different realizations regarding groundwater pollution. The groundwater behaviour can be implemented using a mixture of diffusion and convection equations. The analysis of the convection diffusion equation is also interesting for other research areas, for example biology, chemistry and the stock market. The first part will deal with the derivation of the regarded equation. Then there are different types of approaches which will be used to analyse the behaviour of this equation. On the one hand there are analytical and numerical methods to solve or approximate this partial differential equations. On the other hand a more stochastic approach will be introduced.

Keywords: Diffusion, Mathematical Modelling, Finite Different and Element Method, Cellular Automata

1. INTRODUCTION

The pollution of groundwater is an important field of interest regarding the water supply of all countries no matter how poor or rich. The analysis of this problem is based on the study of partial differential equations. In this case it can be restricted to the analysis of the convection diffusion equation. Diffusion equations are not only used to describe distribution of pollution. In biological fields of studies these equations are used to model the development of pattern formation for example in the fur of cats. There are also other fields which are confronted with the analysis for example of reaction-diffusion equation. In the chemistry the mixture of two substances can be simulated using this equation. Also in the finance market another form of the diffusion equation is used to predict the behaviour of stock buyers. The main point of this paper is a comparison of different methods simulating convection-diffusion equations. There are three different approaches explained. At first a analytical solution is given. Unfortunately this may not be possible in any given scenario. Therefore the second approach deals with numerical methods solving the partial differential equation. In order to evaluate the results of all approaches properly the analytical solution can be used. The third method covers a stochastic approach, well known as Random Walk. In the paper not only the results but also the advantages and disadvantages of the methods are discussed.

The starting point of this research was a Benchmark of EUROSIM. In this Benchmark a rectangle is given. There is a flux along the x–axis which is constant. The given diffusion coefficient is constant as well. Therefore the convection diffusion equation will be analysed in a two dimensional rectangular area with a constant flow along the x–axis.

2. CONVECTION DIFFUSION EQUATION

The needed convection-diffusion equation can be separated in two parts, each describing a different process. One the one hand there is the oriented movement, called the convection. On the other hand there is a chaotic behaviour which describes the diffusive motion. This movement is characterized by minimal randomized motion of small particles. A transport of particles from regions with high concentration to areas with low concentration can be observed. This behaviour is mathematically formalized in Fick's First Law:

$$J_d : \mathbb{R}^n \to \mathbb{R}^n \quad \text{with} \quad J_d(\mathbf{x}) = -D(\mathbf{x}) \cdot \nabla c(\mathbf{x}) \tag{1}$$

It declares that the flux is proportional to the concentration gradient going from regions with high concentration to regions with low concentration as described in Larsson et al. (2005). The variable J_d stands for the diffusive flux. This can be a function of space x. The flux is also influenced by the diffusion coefficient D and the concentration c.

The oriented movement, the convection, accrues due to a flux. The flux is described with a velocity field $\mathbf{v}$. This vector field contains the flow movement in every possible direction. It can, as well as before, depend on space variables. Due to flux velocity the concentration c of a certain substance at point $\mathbf{x}$ will be transported to the place $\mathbf{x}+tv$ after time step t. Therefore the convective flux of mass $J_c : R^n \to R^n$ can be written as:

$$J_c(\mathbf{x}) = v \cdot c(\mathbf{x}). \tag{2}$$

Due to the fact that a closed system is considered the conservation law can be used. In this case it means, that the regarded property does not change. It describes the relation between the time rate of change regarding the concentration of a certain quantity c and the change in space regarding the flux J.

$$\frac{\partial c}{\partial t} + \nabla \cdot J(\mathbf{x}) = 0 \tag{3}$$

The combination of the equations (1) and (2) results in the replacement of the the flux J in equation (3) with $J = J_c + J_d$. This leads to the diffusion equation.

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$$\frac{\partial c}{\partial t} + \nabla \cdot J = 0 \Rightarrow \frac{\partial c}{\partial t} + \nabla\left(-D \cdot \nabla c + v \cdot c\right) = 0 \qquad (4)$$

$$\Rightarrow \frac{\partial c}{\partial t} = \nabla\left(D \cdot \nabla c\right) - \nabla\left(v \cdot c\right) \qquad (5)$$

If the diffusion coefficient and the velocity field are constant the equation can be written as follows:

$$\frac{\partial c}{\partial t} = D \cdot \nabla^2 c - v \cdot \nabla\left(c\right). \qquad (6)$$

Due to the fact that the convection-diffusion equation will be analysed in a two dimensional area the equation of the following form will be needed.

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) - v\frac{\partial c}{\partial x} \qquad (7)$$

Every partial differential equation needs a certain initial condition and if the equation is second order also boundary conditions. In the following analysis two different scenarios will be considered. On the one hand the initial condition can be described using the δ–distribution. This means that there is an initial amount of pollution at the source which will be distributed during time. In the other scenario there is a constant source of pollution.

3. ANALYTICAL SOLUTION

Due to the special initial and boundary condition it is possible to find the analytical solution very easily. In order to solve the two dimensional equation the solution of the one dimensional case should be considered. Below the equation and the conditions for the one dimensional area are given.

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} \quad \text{with} \quad c(x,0) = \delta(x), \quad \lim_{x \to \pm\infty} c(x,t) = 0. \qquad (8)$$

Using a certain substitution, see Schulten et al. (2000), the equation (8) can be transformed to the following form:

$$\tau = Dt, \qquad b = \frac{v}{D} \qquad (9)$$

$$y = x - b\tau, \qquad y_0 = b\tau_0 \qquad (10)$$

$$\frac{\partial c(y,\tau)}{\partial \tau} = \frac{\partial^2 c(y,\tau)}{\partial y^2}. \qquad (11)$$

The multiplication of the equation (11) by $e^{-p\tau}$ and the integration with respect to τ afterwards results in an ordinary differential equation. This equation can be solved with the according theory very easily. Using the inverse Laplace-transformation the resulting solution will be transformed again. After backwards-substitutions the solution of the one dimensional problem can be given.

$$c(x,t) = \frac{1}{\sqrt{4\pi D t}}\,\mathrm{e}^{-\frac{(x-vt)^2}{4Dt}} \qquad (12)$$

In order to solve the following two-dimensional equation

$$\begin{aligned} &\frac{\partial c}{\partial t} = D \cdot \frac{\partial^2 c}{\partial x^2} + D \cdot \frac{\partial^2 c}{\partial y^2} - v \cdot \frac{\partial c}{\partial x} \quad \text{with} \\ &c(x_0, y_0, 0) = \delta(x)\delta(y) \\ &\lim_{x,y \to \infty} c(x,y,t) = 0 \\ &\lim_{x,y \to -\infty} c(x,y,t) = 0 \end{aligned} \qquad (13)$$

a solution of the following form can be assumed as in Zoppou et al. (1999).

$$c(x,y,t) = g_1(x,x_0,t)\,g_2(y,y_0,t) \qquad (14)$$

Whereas the two functions g_1 and g_2 are solutions of the one-dimensional convection-diffusion equation with constant coefficients as seen above. Therefore g_1 and g_2 are the solution of the one dimensional equation(12) which will be formulate for the x– and the y–axis.

$$\begin{aligned} g_1(x,x_0,t) &= \frac{A_1}{2\sqrt{D\pi t}} \exp\left(\frac{-(x - x_0 - vt)^2}{4Dt}\right) \\ g_2(y,y_0,t) &= \frac{A_2}{2\sqrt{D\pi t}} \exp\left(\frac{-(y - y_0)^2}{4Dt}\right) \end{aligned} \qquad (15)$$

The source of pollution is located at the origin of the area. That means that the values x_0 and y_0 can be set to zero. Additionally, due to the initial condition the integral over the whole area has to be 1.

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c(x,y,t)\,dx\,dy = \\ &= \int_{-\infty}^{\infty} g_1(x,0,t)\,dx \int_{-\infty}^{\infty} g_2(y,0,t)\,dy = A_1 A_2 \end{aligned} \qquad (16)$$

This leads to the analytical solution in two dimensions.

$$c(x,y,t) = \frac{1}{4D\pi t}\ \exp\left(\frac{-(x - vt)^2 - y^2}{4Dt}\right) \qquad (17)$$

The implementation of this solution for the two-dimensional case can be shown in the following figure.

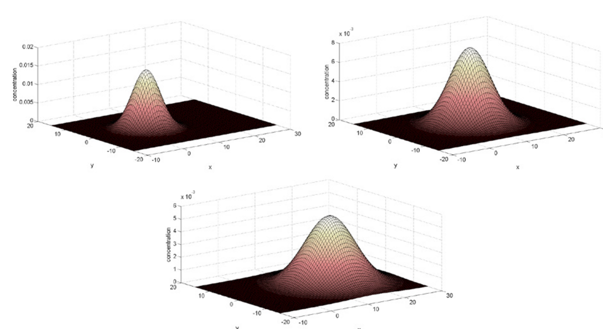

Fig. 1. Two dimensional diffusion using (17) for different time steps $(250, 500, 750$ seconds) is shown.

Figure 1 shows the analytical solution of the convection-diffusion equation for the case of an instantaneous release of all pollution. The used parameter are velocity $v = 0.02$ and diffusion $D = 0.02$: To visualize the behaviour over time different values for the simulation time are chosen, $t = 250s$, $t = 500s$