Different Methods analysing Convection-Diffusion

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Abstract. Many countries in this world have lack of drinking water. Austria has advantage of drinking water coming from the mountains. This article contains a study focusing on mathematical modelling using different methods for the analysis of groundwater pollution. The distribution of pollution follows the convection-diffusion equation. Therefore different methods ranging from analytical and numerical to alternative approaches dealing with random walk are compared. The analysis of the approaches is mostly done for one and two dimensional case.

Introduction

In order to analysis the po llution distribution in water of sim ilar circum stances the m athematical equation describing t his be haviour i s a c onvection-diffusion equation. This equation can not only be used to analysis the be haviour of pollution. Also in biology, chem istry and ot her fiel ds of study t his e quation i s im portant. Regarding biol ogy the equation can be use d to predict the development of fur pattern for cats. In chemistry the mixture of different substances follows this equation. In the field of physical modelling and simulation this equation is often c alled heat equation bec ause it describe s the distribution of heat em anating from a source. De - spite disci plines in nat ural sciences also the fi nance market uses this equation t o foresee the behaviour of buyers of st ocks. In general the convection- diffusion equation looks as follows:

$$\frac{\partial c}{\partial t} = D \cdot \nabla^2 c - v \cdot \nabla c \tag{1}$$

Equation (1) is a partial differential equation of second or der a nd c ontains tw o dif ferent variables D, v which can be ti me-dependent, position-dependent or simply constant. In the following we assume that all the variables are constant. The first term of this equation describes a re gular distri bution in every direction. It is similar to spreading of waves after throwi ng in a little stone into water. The variable v in th e secon d term of (1) symbolises the velocity field of oriente d movement. Assuming for example a river with a ce rtain flux the n the distribution would be influence by the velocity of the flux. This information w ill be transformed into t he equation using the variable v. To sum it up, the convection-diffusion equation contains one part de scribing the chaotic movement in all dir ections and an orie nted distribution depending on the circumstances. In the following a fl ux only in x- direction is assumed. This pr oblem description wi ll be a nalysed usi ng three different a pproaches applied in one and two dimensions.

1 Analytical Solution

In this case, due to the used initial and boundary conditions, an anal ytical solutio n can be given. The initial condition describes a pollutio n sources which releases all the pollution at ti me $t = 0$ without inj ecting any further pollution. B oth so lutions, one- and two-dimensional, are used to validate the different methods.

One-dimensional. Using the regarded equation is given as follows

$$\frac{\partial c}{\partial t} = D \cdot \frac{\partial^2 c}{\partial x^2} - v \cdot \frac{\partial c}{\partial x} \tag{2}$$

and has to fulfill the initial $c(x_0, 0) = \delta(x)$ and the boundary conditions $\lim_{x \to \pm\infty} c(x,t) = 0$. Using substitutions described in [1] the equation (2) can be written as

$$\begin{gathered} \tau = Dt, \qquad b = \frac{v}{D} \\ y = x - b\tau, \qquad y_0 = b\tau_0 \\ \frac{\partial c(y,\tau)}{\partial \tau} = \frac{\partial^2 c(y,\tau)}{\partial y^2} \end{gathered} \tag{3}$$

The resulting line in equation (3) can be multiplied by $e^{-p\tau}$. After integration with respect to τ one obtains an ordinary differential equation which can be solved using basic mathematical tools. A Laplace back transformation and backward substitution gives the solution of equation (2).

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

Two-dimensional. In the two dimensional case the obtained equation changes to

$$\frac{\partial c}{\partial t} = D \cdot \frac{\partial^2 c}{\partial x^2} + D \cdot \frac{\partial^2 c}{\partial y^2} - v \cdot \frac{\partial c}{\partial x} \tag{5}$$

Analogue to the one-dimensional case certain initial and boundary conditions are defined as follows

$$c(x_0, y_0, 0) = \delta(x)\delta(y)$$
$$\lim_{x,y\to\infty} c(x,y,0) = 0$$
$$\lim_{x,y\to-\infty} c(x,y,0) = 0$$

In order to solve equation (5) a specific form of the solution is assumed.

$$c(x,y,t) = g_1(x,x_0,t)g_2(y,y_0,t) \tag{6}$$

The functions g_1 and g_2 are solutions of the one-dimensional convection- diffusion equation with constant coefficients. Therefore g_1 and g_2 can be taken from the one-dimensional analytical solution (4).

$$\begin{aligned} g_1(x,x_0,t) &= \frac{A_1}{2\sqrt{D\pi t}} e^{-\frac{(x-x_0-vt)^2}{4Dt}} \\ g_2(y,y_0,t) &= \frac{A_2}{2\sqrt{D\pi t}} e^{-\frac{(y-y_0)^2}{4Dt}} \end{aligned} \tag{7}$$

The source is located at the origin therefore the values $x_0 = 0$ and $y_0 = 0$ can be inserted. Additionally the integral over the whole domain has to be 1.

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c(x,y,t) = \\ &= \int_{-\infty}^{\infty} g_1(x,0,t)dx \int_{-\infty}^{\infty} g_2(y,0,t)dy = A_1A_2 \end{aligned} \tag{8}$$

This integration result leads to the analytical solution in two dimensions.

$$c(x,y,t) = \frac{1}{4Dt\pi} e^{-\frac{(x-vt)^2}{4Dt}} \tag{9}$$

2 Numerical Approximation

This section introduces two types of numerical approximations. On the one hand there is the finite difference method (FDM). In this approximation the derivative of the differential equation is approached by taking the difference quotient of the neighboring grid points. The method is easy to use but slightly weak concerning the accuracy. The second method is the finite element method (FEM) and is based on formulating variations of the differential equation. FEM determines approximated solutions consisting of piecewise defined polynomials on a fine resolution of the domain. The advantage of FEM is the suitability for any geometry.

2.1 Finite Difference Method

One-dimensional. Using finite differences to approximate the first and second derivatives the partial differential equation (2) transforms into an ordinary differential equation.

$$\frac{dc}{dt} = D \cdot \frac{c_{i+1} - 2c_i + c_{i-1}}{dx^2} - v \cdot \frac{c_i - c_{i-1}}{dx} \tag{10}$$

The time derivative can be replaced as follows

$$\frac{dc}{dt} = \frac{c^{k+1} - c^k}{\Delta t} \tag{11}$$

Using (11) equation (10) can also be written as a matrix product

$$\frac{c^{k+1} - c^k}{\Delta t} = S \cdot c^k \tag{12}$$

whereas c^k is the current concentration of pollution and c^{k+1} the concentration in the next time step. In order to determine c^{k+1} using the Explicit Euler equation (12) is rearranged.

$$c^{k+1} = (S \cdot \Delta t + I)c^k \tag{13}$$

It is well known that the Explicit Euler can be unstable using the wrong step size relation. Notation (12) can be also used to find the Implicit Euler formulation. The current concentration on the right hand side in equation (13) is replaced by the concentration of the future time step in order to obtain the implicit formulation.

$$c^{k+1} = (I - S \cdot \Delta t)^{-1}\, c^k \tag{13}$$

Two-dimensional. Regarding the problem formulation in two dimensions the finite difference method looks a little bit different. Due to the fact that an equidistant grid, $dx = dy$ is used the approximation can be given as follows

$$\begin{aligned} \frac{dc}{dt} = D \cdot &\frac{c_{x+1,y} + c_{x-1,y} - 4c_{x,y} + c_{x,y+1} + c_{x,y-1}}{dx^2} \\ &- v \cdot \frac{c_{x,y} - c_{x-1,y}}{dx} \end{aligned} \tag{14}$$

In contrary to the two-dimensional case the matrix notation is not as easy as in one dimension.

$$c_{x,y}^{k+1} = c_{x,y}^{k} + h\frac{dc}{dt} \tag{15}$$

Therefore only the Explicit Euler method is implemented as shown in (15).

2.2 Finite Element Method

The finite element method was only realized for the convection-diffusion equation in one dimension.

$$\begin{gathered}\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial t^2} + v\frac{\partial c}{\partial x} = 0 \text{ in } \Omega \\ c = 0 \text{ on } \partial\Omega\end{gathered} \tag{16}$$

First of all the weak solution of (16) is formalized using a test function of the according Sobolev space $\phi \epsilon H_0^1$.

$$\int_\Omega \frac{\partial c}{\partial t}\phi \, d\Omega + \int_\Omega (D\,\nabla c\,\nabla\phi + v\nabla c\,\phi) = 0 \tag{17}$$

The formulation of the Galerkin approximation is necessary to formulate the solution equation of the finite element method.

$$c^n(x) = \sum_{j=1}^{n} c_j\varphi_j(x) + c_0(x) \tag{18}$$

The unknown variables c_j in equation (18) have to be determined. Using linear basis functions called 'hat-functions' for φ a linear system of n equations with n unknowns, called the Galerkin formulation, results [3].

$$\begin{gathered}\sum_{j=1}^{n_e}\frac{\partial c_j}{\partial t}\int_{\Omega^{e_k}}\varphi_i\,\varphi_j\,d\Omega + \\ \sum_{j=1}^{n_e} c_j\int_{\Omega^{e_k}}(D\,\nabla\varphi_j\,\nabla\varphi_i + \nabla\varphi_j\,\varphi_i)\,d\Omega = 0\end{gathered} \tag{19}$$

In equation (19) n_e is the number of elements in every finite element and Ω^{e_k} is the domain of element e_k. Equation (19) can also be written in a short form.

$$\begin{gathered}\dot{c}\cdot M + c\cdot S = 0 \\ m_{ij} = \int_{\Omega^{e_k}}\varphi_i\,\varphi_j\,d\Omega \\ s_{ij} = \int_{\Omega^{e_k}}(D\,\nabla\varphi_j\,\nabla\varphi_i + \nabla\varphi_j\,\varphi_i)\,d\Omega\end{gathered} \tag{20}$$

The matrices of (20) are called mass matrix M and stiffness matrix S. Considering the mentioned 'hatfunctions' it is clear, that only a few of the possible integrals are not equal zero.

Those basis functions which correspond to the corner points of the element will lead to non trivial results. Because the element i is connected to $i-1$ and $i+1$ the profile of the matrices is a band matrix with width three.

$$\begin{gathered}M\frac{c^{k+1} - c^k}{\Delta t} + \theta S c^{k+1} + (1-\theta)S c^k = 0 \\ 0 \le \theta \le 1\end{gathered} \tag{21}$$

Equation (22) is called θ-method and will be used to present implicit and explicit methods for solving (21). The most common values for q are:

- $\theta = 0$, Eplicit Euler
- $\theta = 1$, Implicit Euler
- $\theta = \frac{1}{2}$, Implicit Heun

Using this method the Explicit and Implicit Euler algorithm can be given.

$$\begin{gathered}c^{k+1} = M^{-1}(M - \Delta t S)c^k \\ c^{k+1} = (M + \Delta t S)^{-1} M\, c^k\end{gathered} \tag{22}$$

3 Random Walk

An alternative method for simulating transport is the so-called random walk. This approach is contrary to the numerical solutions. The focus changes from a macroscopic view to the simulation of microscopic behavior of diffusion by analyzing movements of single particles.

3.1 Intuitive Approach

The intuitive approach describes a model which uses no grid or collision rules. It is implemented again for both dimensions.

One-dimensional. At the beginning t = 0 all the particles are placed in the origin presenting the source of pollution. The pollution injection happens only at t = 0. The simulation focuses on the convection and diffusion behaviour of these initial particles. In this approach the movement of particles is described by:

$$\begin{gathered}p_{new} = p_{old} \\ r = X\cdot\Delta x\end{gathered} \tag{23}$$

The particle motion in (23) consists of three parts. In order to get the new position p_{new} at time $t + \Delta t$ these three components are summed up. The variable p_{old} stands for the position at time t. The velocity field v is multiplied by the step size. The variable r describes the diffusive movement of a particle for one time step and is added to the former particle position p_{old}.

The second equation in (23) defines the movement r in particular. It consists of the step size in space Δx and a normally distributed random variable X with mean zero and unit variance. In every time step the new position of every particle is calculated with equation (23).

The simulation ends when the chosen simulation time tend is reached.

Two-dimensional. For expansion in a two-dimensional domain the movement has to be defined in a different way. There is no initial velocity but there is an initial direction of every particle d_0. The diffusive transport is realized by using a normally distributed random variable X and a uniformly distributed random number U. X is used to generate a random length and U chooses a coincidental direction.

$$r = X \cdot \Delta x \qquad \alpha = U \cdot 2\pi$$
$$d_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad d_{n+1} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \cdot d_n \tag{24}$$

In (24) r stands for the distance the particle moves in a certain time step. The influence of this parameter is similar to the diffusion coefficient. X is the mentioned normally distributed random variable and Δx describes the step size in space. The second equation of (24) sets the direction for the particle's next move. The initial direction d_0 is only necessary for the recursive definition. During simulation the direction of the last movement is used to calculate the next one. The convection is realized by a shift in flow direction along x. The final formulation of the random walk movement can be given as follows

$$p_{new} = p_{old} + d \cdot r + v\,\Delta t \tag{25}$$

3.2 Gaussian Approach

This approach shows the connection between a random walk approach and the analytical solution.

One-dimensional. The analytical solution of the convection-diffusion equation (2) is used to define the particle movement. Considering the probability density function of a normal or Gaussian distribution

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{26}$$

At the beginning t = 0 all the particles are placed in the origin presenting the source of pollution. The pollution injection happens only at t = 0 . The simulation focuses on the convection and diffusion behaviour of these initial particles. In this approach the movement of particles is described by:

$$\begin{gathered} \mathrm{p_{new}} = \mathrm{p_{old}} \\ r = X \cdot \Delta x \end{gathered} \tag{27}$$

the formal equivalence to the analytical solution (4) is obvious. The parameters used in (27) stand for the mean value m and the standard deviation s which characterize the position and the width of the Gaussian bell curve in a unique way. Therefore the according parameters in (4) can be read out. [4]

$$\mu = v \cdot t \qquad \sigma^2 = 2 \cdot Dt \tag{28}$$

Due to the properties and meaning of the parameters in (28) the height and width of the concentration peak depending on time is given. The corresponding particle movement using (29) can be formulated as follows

$$p_{new} = p_{old} + v\,\Delta t + \sqrt{2D\Delta t} \cdot X \tag{29}$$

The variable X stands for a normally distributed random number with mean zero and unit variance as in the intuitive approach. X is newly generated in every step for each particle. Identifiable by the velocity v the second term stands for the convective motion. This term is equal to the term of the intuitive approach. The radical term describes the diffusive motion and is based on the standard derivation.

Two-dimensional. In order to enlarge this approach in two dimensions the movement along y-direction has to be added. For an expansion in a two-dimensional domain the y-component of the movement has to be defined. Due to the fact that there is no flux the new particle position can be calculated using

$$\begin{aligned} p_x^{new} &= p_x^{old} + v\,\Delta t + \sqrt{2D\Delta t} \cdot X_x \\ p_y^{new} &= p_y^{old} + \sqrt{2D\Delta t} \cdot X_y \end{aligned} \tag{30}$$

The variables X_x and X_y stand for independent normally distributed random numbers which are newly generated in every step for each particle. The term $v\Delta t$ describes the convective transport. Due to the fact that the diffusion coefficient is equal for the x- and y-direction the diffusive movement $\sqrt{2D\Delta t}$ in the random walk definition (30) is the same.

4 Results

In the following section the analytical solutions in both dimensions are compared to the various approaches. The different concentration errors are discussed. In general the parameter setting is: diffusion coefficient $D = 0.02$ and velocity $v = 0.02$.

The step sizes Δt and Δx are variable. The regarded simulation time varies between $t_{end} = 250$ and $t_{end} = 500$.

4.1 Analytical vs. Finite Difference Method Results

First of all the numerical solutions are considered.

One-dimensional. In the plot below in Figure 1 the red curve i s the analyti cal solution and the blue line sketches the numerical approximation using the Implicit Euler algorithm.

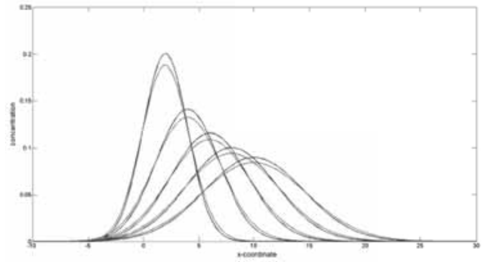

Figure 1. Comparison of the analytical solution and FDMusing matrix notation.

The results in Table 1 show the instability of the Explicit Euler m ethod. The I mplicit Euler algorithm is not only ultra-stable but also faster and more exact than the Explicit Eu ler. The a pproximation u sing finite differences is well-fitting.

		Explicit Euler		Implicit Euler	
Δt	Δx	$\lVert\cdot\rVert_\infty$	$\lVert\cdot\rVert_1$	$\lVert\cdot\rVert_\infty$	$\lVert\cdot\rVert_1$
1	1	0.016	$4.231E^{-4}$	0.016	$4.753E^{-4}$
1	$\frac{1}{2}$	0.009	$1.404E^{-4}$	0.010	$1.600E^{-4}$
$\frac{1}{2}$	$\frac{1}{4}$	0.005	$0.831E^{-5}$	0.005	$7.323E^{-5}$
$\frac{1}{2}$	$\frac{1}{16}$	NaN	NaN	0.002	$3.531E^{-5}$

Table 1. Error values of FEM using Explicit and Implicit Euler.

Two-dimensional. The results re garding t he two-dimensional im plementation show a similar behaviour. In the following the error values are studied in detail.

Also in the two-dimensional case the Explicit Euler works not for all parameter choices. The error values are again quite good. Th e finite d ifference meth od of th e two-dimensional dom ain approximates the convec tion-diffusion equation in an appropriate way.

		Explicit Euler	
Δt	Δx	$\lVert\cdot\rVert_\infty$	$\lVert\cdot\rVert_1$
1	1	0.027	$1.5624E^{-4}$
1	$\frac{1}{2}$	0.017	$3.779E^{-5}$
$\frac{1}{2}$	$\frac{1}{4}$	$9.148E^{-4}$	$1.464E^{-5}$
$\frac{1}{4}$	$\frac{1}{8}$	$.E^{119}$	$.E^{120}$

Table 2. The error values for FDM are shown.

4.2 Analytical vs. Finite Element Method Results

The accuracy of the finite element method is better than of the finite difference method.

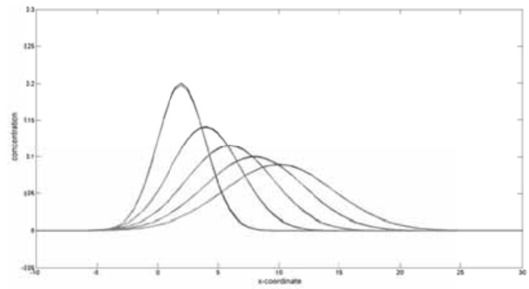

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Figure 3. The error for the Implicit Euler algorithm of the FEM is shown.

In Figure 3 above the upper plot shows t he analytical solution as well as the fi nite element method using Implicit Euler. It is hard to distinguish the different curves.

		Explicit Euler		Implicit Euler	
Δt	Δx	$\lVert\cdot\rVert_\infty$	$\lVert\cdot\rVert_1$	$\lVert\cdot\rVert_\infty$	$\lVert\cdot\rVert_1$
1	1	$7.18E^{-4}$	$3.16E^{-5}$	$9.95E^{-4}$	$3.03E^{-5}$
1	$\frac{1}{2}$	$6.23E^{-4}$	$8.60E^{-5}$	$6.09E^{-4}$	$8.54E^{-5}$
$\frac{1}{2}$	$\frac{1}{4}$	$3.13E^{-4}$	$1.02E^{-4}$	$2.74E^{-4}$	$1.01E^{-4}$
$\frac{1}{4}$	$\frac{1}{8}$	NaN	NaN	$2.49E^{-4}$	$1.05E^{-4}$

Table 3. Depending on the used FEM error values are shown.

The instability of the Implicit Euler is shown in the last row of table 3. In general the error results are smaller compared to the results o f the finite diffe rence method in one dim ension. The finite element me thod approximates the conve ction-diffusion equation better than the finite difference method.

4.3 Analytical vs. Stochastic Results

The accuracy of the random walk approaches is discussed in the following paragraph.

One-dimensional. In the plot below in Figure 1 the red curve is the analytical solution and the blue line sketches the numerical approximation using the Implicit Euler algorithm.

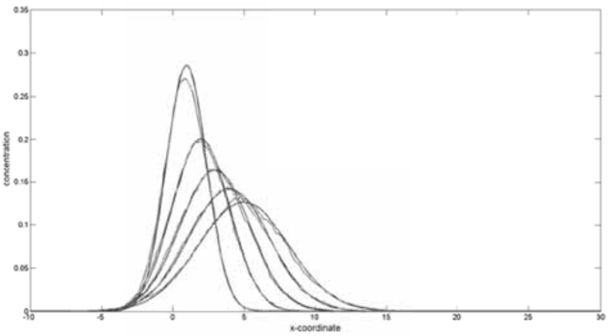

Figure 4. Results of stochastic based random walk are shown.

The graphic in Figure 4 show the Gaussian random walk approach coloured in red and the analytical solution in blue. In the numerical comparisons the simulation time is $t_{end} = 500s$. Due to long execution times for the particle movement this parameter is reduced to $t_{end} = 250s$. The diffusion coefficient is usually set to $D = 0.02$ but modifies if the intuitive approach is used.

Δt	Δx	Gaussian $\|.\|_\infty$	Random Walk $\|.\|_1$
1	$\frac{1}{5}$	0.012	$8.948E^{-7}$
1	$\frac{1}{10}$	0.008	$9.707E^{-7}$
$\frac{1}{2}$	$\frac{1}{5}$	0.007	$8.948E^{-7}$
$\frac{1}{2}$	$\frac{1}{10}$	0.010	$9.707E^{-7}$

Table 4. Comparison of random walk analytical solution.

The Table 4 shows all the error results of the parameter study comparing the analytical solution and the random walk. The diffusion coefficient for the Gaussian-based algorithm is set to $D = 0.02$. Regarding simulation of the convection-diffusion equation, the implementation of the Gaussian-based random walk fits better than the intuitive approach. The number of particles is 6000.

Two-dimensional. In order to compare the analytical solution to a random walk approach the results have to be adapted. In the random walk the output describes the smoothed amount of particles in every cell. Due to the initial Dirac-function the integral at the beginning has value one. The area of the random walk domain is discretizised. Therefore the output has to be divided not only by the number of particles but also by the area of the cells used for the flattening. Table 5 shows the approximation results. The parameter r describes the used radius for the flattening. If the spatial step size is decreasing a greater radius r can be used. If r is chosen too big compared to Δx the result loses the shape of a bell curve. Compared to the results of the numerical simulation the random walk approach leads to greater error values. The number of particles is 4000.

Δt	Δx	r	N	Implicit $\|.\|_\infty$	Euler $\|.\|_1$
1	1	3	4000	$3.395E^{-3}$	$6.349E^{-4}$
1	$\frac{1}{2}$	8	4000	$5.033E^{-3}$	$3.737E^{-5}$
$\frac{1}{2}$	$\frac{1}{4}$	15	4000	$4.526E^{-3}$	$1.005E^{-4}$
$\frac{1}{2}$	$\frac{1}{8}$	20	4000	$2.801E^{-3}$	$2.206E^{-3}$
1	$\frac{1}{4}$	20	8000	$6.764E^{-3}$	$1.826E^{-4}$

Table 5. Comparison of random walk analytical solution.

5 Conclusion

In general the finite element method approximates the convection-diffusion equation the best. Of course the very best solution is the analytical one. In spite of it all random walk approaches are quite good approximations of the convection-diffusion equation.

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