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.

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

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

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

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

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.

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

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.

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

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

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

$$y = x - b\tau, \qquad y_0 = b\tau_0 \tag{10}$$

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

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.

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

In order to solve the following two-dimensional equation

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

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

$$c(x,y,t) = g_1(x,x_0,t) g_2(y,y_0,t) \tag{14}$$

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.

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

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.

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

This leads to the analytical solution in two dimensions.

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

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

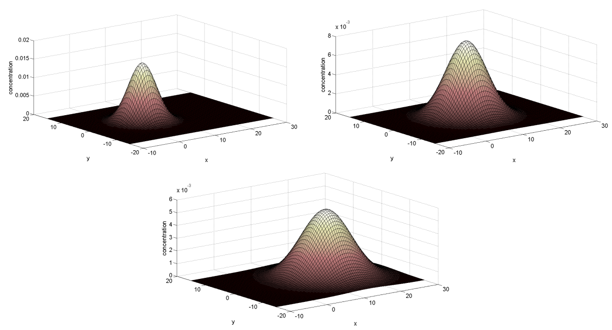

Fig. 1. Two dimensional diffusion using (17) for different time steps $(250, 500, 750$ seconds) is shown.

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, $t = 250s$, $t = 500s$

and $t = 750s$. The three correspondent graphics show show the concentration as a function of x and y. On the one hand the movement according to the flux along the x–axis is obvious. The peak in the first figure is located at $x = 5$, for the second at $x = 10$ and for the last one at $x = 15$. Also the influence of the diffusion coefficient is visible. Altough the figures show different sclaes on the third axis the height values can be given. The peak of the curve starts at 0.035, goes to 0.016 and ends at 0.012. The choice of the parameter shows a good balance between convective and diffusive transport.

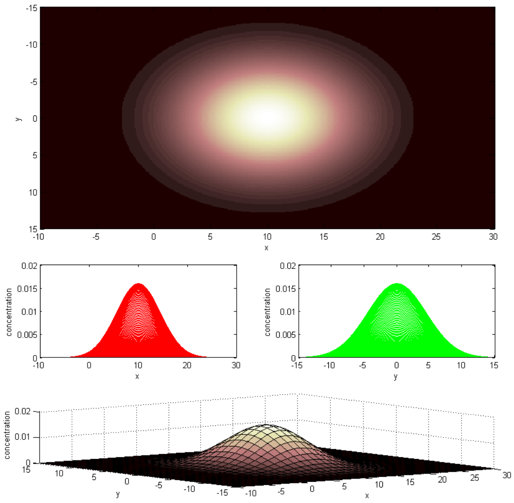

Fig. 2. Analytical solution of equation (17) on the rectangle.

Figure 2 shows three different aspects of the analytical solution. The two plots in the middle of the figure sketch the diffusive progress from the x– and y–axis point of view. The red one shows the convection of the concentration peak moving from $x = 0$ at the beginning to $x = 10$ at the end. The peak of the green bell curve is still at $y = 0$ because there is no velocity along the y-direction. The lowest plot shows the concentration dependent on x and y as in Figure 1, which offers a three dimensional view of the red and green curves. The uppermost illustration can be seen as the aerial perspective of the third graphic. The different colors mark the grade of pollution. The duration of this simulation is $t = 500s$. All other parameters are the same as in figure 1, velocity $v = 0.02$ and the diffusion coefficient $D = 0.02$.

4. 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 derivatives of the partial differential equation are approximated by taking the difference quotient of the neighbouring 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 its suitability for any geometry.

4.1 Finite Difference Method

The finite difference method for one dimension can be explained easily. Instead of the first derivative of the function the differential quotient of neighbouring points is used. In order to receive the second derivative this procedure is applied on the resulting first derivative of neighbouring points. The same principle is used to apply the finite difference method for a two dimensional domain. Consider the finite domain covered with an equidistant grid.

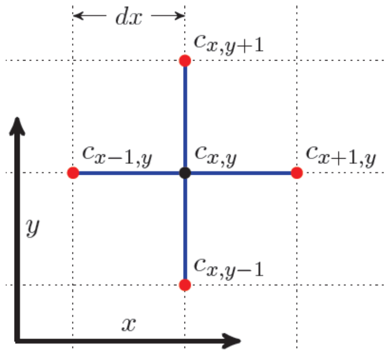

Fig. 3. Equidistant grid in the two dimensional domain.

Considering the principle of the one dimensional finite element method explained above one can imagine how the first partial derivatives of the function $c(x,y)$ look like, shown in equation (18).

$$\frac{\partial c}{\partial x} = \frac{c_{x+1,y} - c_{x-1,y}}{2dx}$$
$$\frac{\partial c}{\partial y} = \frac{c_{x,y+1} - c_{x,y-1}}{2dy} \qquad (18)$$

To establish second derivatives again the central finite difference is used. Repeating the finite difference for the first derivative of two neighbouring points it results into the second derivative for variable x of $c(x,y)$. The partial derivatives for y can be defined analog. Combining these two equations and assuming the usage of a equidistant grid, which means $dx = dy$, one receives the needed form of the second derivation and the Laplace operator.

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_{x+1,y} - 2c_{x,y} + c_{x-1,y}}{dx^2}$$
$$\frac{\partial^2 c}{\partial y^2} = \frac{c_{x,y+1} - 2c_{x,y} + c_{x,y-1}}{dx^2} \qquad (19)$$
$$\Rightarrow \Delta c = \frac{c_{x+1,y} + c_{x-1,y} - 4c_{x,y} + c_{x,y+1} + c_{x,y-1}}{dx^2}$$

For simulating the convection-diffusion equation an approximation of the convection is necessary. Due to the fact that the velocity field is only parallel to the x-axis the convection consists of the first derivative only in x as explained and defined in equation (18). The concentration c depends on the spatial coordinates as well as time. Hence, the equation (13) using FDM can be written as:

$$c_t = \frac{dc}{dt} = D \cdot \frac{c_{x+1,y} + c_{x-1,y} - 4c_{x,y} + c_{x,y+1} + c_{x,y-1}}{dx^2} - v \frac{c_{x,y} - c_{x-1,y}}{dx} \quad (20)$$

In (20) the time derivative can be written with dt instead of ∂t because the finite difference method transforms the equation into an ordinary differential equation. The numerical method which is used to calculate the next time step is called explicite Euler method. This method calculates the next time step by using the last one and adding the derivative of the function times step size h.

$$c_{x,y}(t+\Delta t) = c_{x,y}(t) + h \cdot \frac{dc}{dt} \quad (21)$$

The equation (20) is implemented in MATLAB using the explicit Euler method (21).

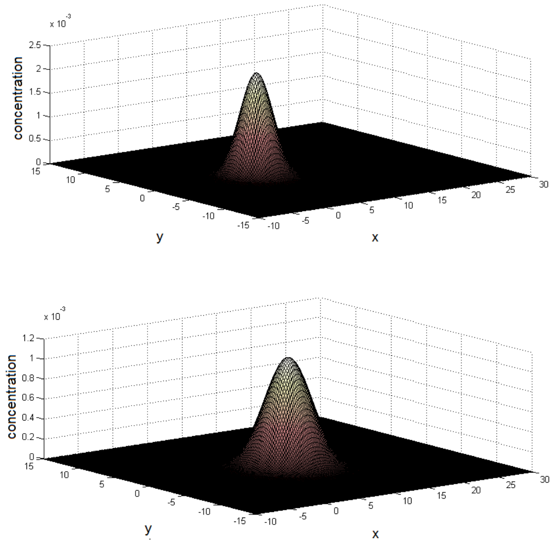

Fig. 4. Numerical solution using FDM for a two-dimensional domain with instantaneous source.

For Figure 4 the parameter setting is: velocity $v = 0.02$, diffusion coefficient $D = 0.02$ and the duration time is $t = 250s$ left and $t = 500s$ right. Therefore the diffusion and velocity coefficient are similar to the analytical results. The same parameters are used to enable comparability. In the first figure the centre of pollution after $250s$ can be found at $(x,y) = (5,0)$ and the height is approximately $c(5,0) = 1.8$. The second plot shows the same parameter set running for $500s$. The height decreases and the centre of peak changes to $(x,y) = (10,0)$. The convective movement is exactly the same as in the analytical solution.

As mentioned at the beginning different initial scenarios are simulated. In the following the source changes from an instantaneously to a steady releasing source. The steady source of pollution is realized by adding partial pollution to the concentration value at $(0,0)$ which leads to $c_{0,0} = c_{0,0} + p_{rate} \cdot \Delta t$ in every time step, whereas p_{rate} stands for the constantly added pollution rate.

The velocity and diffusion coefficient in figure 5 are $v = 0.02$ and $D = 0.02$. They are equal to the parameters in figure

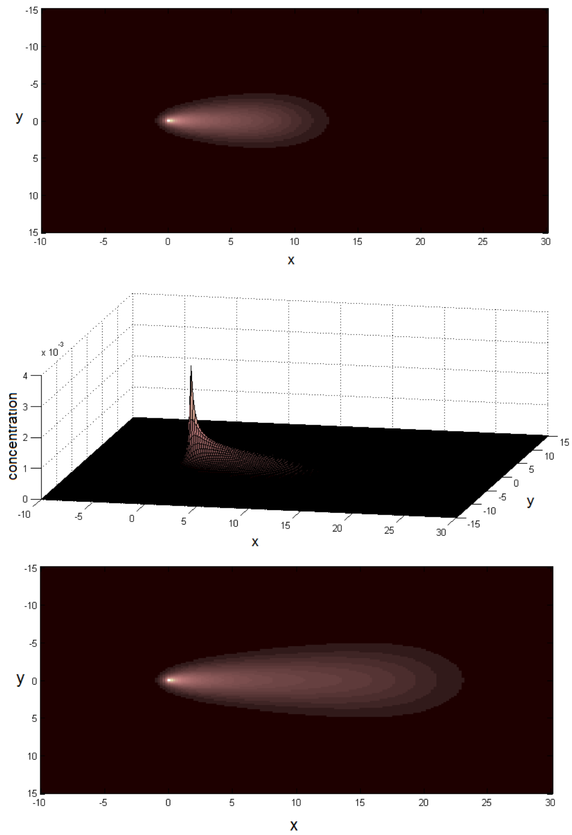

Fig. 5. Numerical solution using FDM for a two-dimensional domain with steady source.

1. The pollution rate was set to $p_{rate} = \frac{1}{t_{end}}$. In doing so the same amount of pollution as in the simulations with in instantaneous source is distributed. In first two images the running time is $t_{end} = 500s$ and in the third $t_{end} = 1000s$. Regardless of how long the simulation runs the maximum of pollution is always at the source itself. The influence of the flux is obvious. The absence of flow in y-direction causes a cone-shaped pollution in x-direction. The upper graphic shows again a colour map of the grade of pollution. The steep peak in the second illustration pictures that the pollution rate added every time step is bigger than the moved pollution due to the convective motion. Therefore some pollution stays near the source for minimal one more time step which causes this peak. Using a longer simulation time the cone gets longer. The pollution particles reaches till $x = 13$ for $t_{end} = 500s$ and around $x = 23$ for the double time span $t_{end} = 1000s$.

4.2 Finite Element Method

Numerical approaches need much computing time due to the need of high accuracy and the requirement of useable outputs. The finite element method for two-dimensional regions is more complicated than for one dimension. Putting a grid on the domain expanses the number of elements to the power of two. For the basis function a linear or quadratic approximation can be used. A direct implementation of the algorithms in MATLAB would be very time-consuming. Instead the software called COMSOL, formerly FEMLAB, is used. It is qualified for physical simulations and is based on the interaction of differential equations. The actual solving algorithm of COMSOL uses the finite element method.

As already mentioned COMSOL offers many different toolboxes. In this case the mathematical package without any additional physical specification is used. In the next step the obtained geometry has to be designed. In this study it is only a rectangular but in case of an natural application it can be necessary to upload a difficult geometry. Therefore the connection to graphical design programs can be used and to import the exact data. The global variables, including the diffusion and velocity coefficient can be defined and stored. The mathematical toolbox offers some prepared equations. The convection-diffusion equation in the following form (22) is one of them.

$$\frac{\partial u}{\partial t} + \nabla(-D\nabla u) + v\nabla u = f \tag{22}$$

The point source is located at $(0,0)$. For the following simulations the function f is set to zero. The simulation time for all parameter choices is $t_{end} = 500$ and the concerning $\Delta t = \frac{1}{4}$. Before the simulation starts the regarded domain is covered with a fine grid 6.

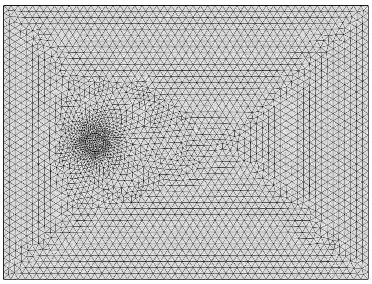

Fig. 6. Grid used in the FEM calculations.

This grid adapts to the certain conditions. The element size is chosen very small to avoid mathematical errors at critical points. Due to the fact that a point source is used the grid refines at its location, which means at $(0,0)$.

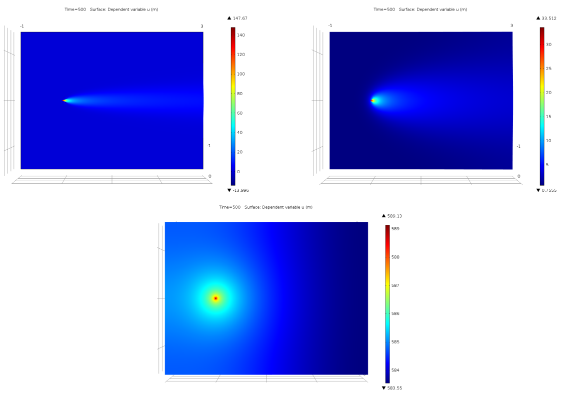

Fig. 7. FEM solution realized using COMSOL.

Figure 7 shows the simulation of the convection-diffusion equation using the software COMSOL. The based method is the finite element method. In the first plot the parameters are set to $D = 0.02$ and $v = 2$. The velocity dominates the diffusive motion. Therefore the concentration distribution shape is only a beam and the pollution reaches the right end of the plotted area. Due to the fact that COMSOL can distinguish different physical meanings of the equation the same variables have another effect to the visualization. In the second graphic the diffusion

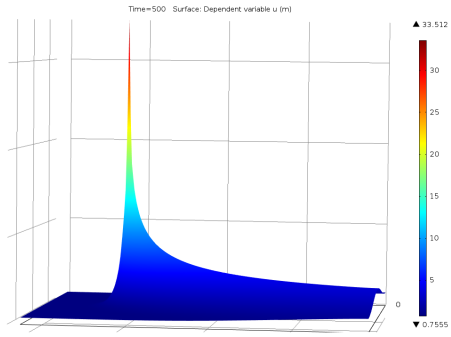

Fig. 8. A surface plot of the COMSOL results is shown.

coefficient is changed to $D = 0.2$. The results look more like the numerical solution outputs achieved with the FDM.. The convection is still dominating but also the diffusive effect can be seen. In the third plot the relation between diffusion and convection is completely different. The parameter are set $D = 2$ and $v = 1$. This parameter choice already shows the domination of diffusion. In the graphic the effects of convection nearly disappears.

Figure 8 shows the second plot of firgue 7 from another angle. The pollution distribution from the x–axis point of view is pictured. Due to the different physical interpretation this solution is not compared to any other approach. For prospective studies COMSOL will play an important role. Especially for complex geometries it is a very comforting application.

5. GAUSSIAN-BASED APPROACH

Conventional numerical methods need a very high grid resolution and in addition a small time step to generate useable results. This leads to long execution times even with the available computer performance nowadays. This problem also occurs regarding the simulation of diffusion.

All the numerical methods describe the convection-diffusion in a macroscopic way. An alternative for simulating transport is the use of random walk. This approach is contrary to the numerical solutions before. The focus changes to the microscopic behaviour of diffusion by analysing single particles. Probability theory is an important basis of random walk. The following solution is implemented without using any grid. The velocity field is chosen to be constant. As in the analytical and numerical simulations it is independent from the particle's position.

The random walk implementation is connected to the two-dimensional analytical solution (17) of the diffusion equation with the following initial and boundary conditions.

$$\begin{aligned} \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} \qquad \text{with} \quad & c(x,0) = \delta(x) \\ & \lim_{x,y\to\pm\infty} c(x,y,t) = 0 \\ & \lim_{x\to\infty}\lim_{y\to-\infty} c(x,y,t) = 0 \\ & \lim_{x\to-\infty}\lim_{y\to+\infty} c(x,y,t) = 0 \end{aligned} \tag{23}$$

Looking at the simplified but differently arranged analytical solution (17)

$$c(x,y,t) = \frac{1}{2\sqrt{D\pi t}} \exp\left(\frac{-(x-vt)^2}{4Dt}\right) \frac{1}{2\sqrt{D\pi t}} \exp\left(\frac{-y^2}{4Dt}\right) \tag{24}$$

the equation parts belonging to the movement along x on the one hand and y on the other hand become visible. Once more the connection to the Gaussian distribution is obvious.

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

There is a formal equivalence regarding parts of the equation (24). The parameters for the mean value μ and the standard deviation σ can be extracted.

$$\mu = v \cdot t$$
$$\sigma^2 = 2 \cdot Dt$$

Therefore the concentration can be approximated using the information of height and width given by the Gaussian parameters. The corresponding particle movement in x and y-direction can be defined as in (25), see Winkler (2014).

$$\begin{aligned} p_x^{new} &= p_x^{old} + v\Delta t + \sqrt{2 \cdot D\Delta t} X_x \\ p_y^{new} &= p_y^{old} + \sqrt{2 \cdot D\Delta t} X_y \end{aligned} \tag{25}$$

X_x and X_y are independent normally distributed random numbers which generated in every step for each particle. The convection is included in the variable $v\Delta t$ and is only necessary in the x related equation. Due to the fact that the diffusion coefficient constant and additionally equal for the x- and y-direction the diffusive movement is characterised trough the term $\sqrt{2 \cdot D\Delta t}$ in (25). It is the same term for both directions.

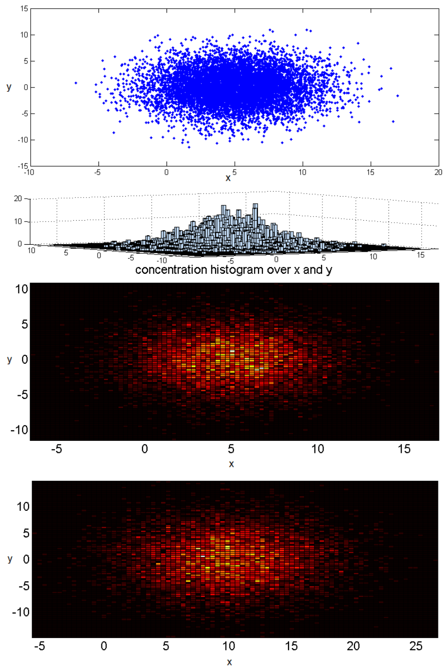

Fig. 9. Gaussian random walk for convection-diffusion with instantaneous releasing source

In Figure 9 two results of the implementation are shown. The parameters are similar to the intuitive approach to enable comparability. This means that the setting is $v = 0.02$ for the velocity and $D = 0.02$ for the diffusion coefficient. The other two variables are set $N = 8000$ which stands for the number of particles and the time step $\Delta t = 1$. The spatial step size $\Delta x = 1$ is used to calculate the velocity part for every time step. The simulation time is set $t = 250$ in the first graphic and $t = 500$ in the second. The first figure consists of three partial plots. The first one shows the position of all used pollution particles. In the second one the histogram of the pollution distribution is pictured. The third one combines the first two. On the one hand the locations of the particles are visible. The additional colour scale shows the density of the particles in the certain area. For the second simulation time only the combined sight is shown. The centre of concentration is equal to the results of the analytical and numerical solutions. The progressive diffusion shows the influence of the diffusion coefficient.

This approach is also used to approximate the convection-diffusion equation in case of a steady polluting source. This is realized by releasing $\frac{N}{t_{end}\frac{1}{dt}}$ particles every time step.

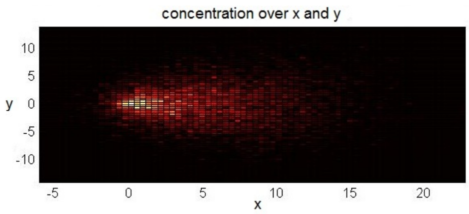

Fig. 10. Gaussian random walk for convection-diffusion with steady source

6. DISCUSSION AND CONCLUSION

The three approaches show the possible variety of implementations regarding the convection diffusion equation. In order to pick the best approximation different circumstances have to be minded. Regarding the programming effort the Gaussian approach is the easiest and quickest possibility. Another advantage is also a flexible geometry of the area. The results are acceptable. The FEM based realisation has the highest accuracy. Compared to the other two approaches the theory is more complex. Therefore it also offers different kinds of realization. The finite difference method has a disadvantage regarding complex geometry and is the slowest implementation. All in all a useful approximation of the general behaviour can be given in all realizations. Further studies regarding analytical approximations for the steady source problem and new methods or implementations will be examined.

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