

Comparison of Finite Difference Method and Random Walk Method in ARGESIM Benchmark C19 'Pollution in Groundwater Flow'

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Abstract. Groundwater represents one of the most important sources so as to satisfy the steadily increasing demand of pure water in modern times. However, groundwater is very susceptible to many kinds of pollution whose causes can usually be divided into one of two categories: point-source and nonpoint-source pollution. In this comparison a particular focus was put on the modelling of a 2D-homogeneous groundwater body and the contamination of its groundwater stream caused by a steady point-source pollution in case of a uniform pore-water velocity. Three different tasks were regarded: In task A, the pollution propagation was investigated and compared to an approximated analytical solution in case that no treatment plants are installed. In contrast, task B and C consisted of examining the impact of treatment plants on the actual pollution propagation in case of a permanent activation and when the pollution reduction works according to a set schedule instead. In total, two different computational approaches were chosen and implemented in Matlab whereby one consisted of a finite difference method and the other was based on a random walk ansatz. Similar results were obtained but further parameter studies could be helpful.

1 Modelling & Task Definition

The modelling in this comparison is restricted to the 2D-description of the pollution propagation within a homogeneous groundwater body which suffers a continuous pollution by a point-source. Hence, from another perspective, it is assumed that the actual groundwater body

can be approximated by a 2D-domain whereby the concentration in z -direction does not differ. Furthermore, the associated groundwater stream shall be characterized by a uniform velocity. For this setting the propagation of the pollution concentration $c = c(x, y, t)$ with unit g/m^2 can be described by the 2D transport equation

$$\frac{\partial c}{\partial t} = \alpha |\mathbf{u}| \nabla^2 c - \mathbf{u} \cdot \nabla c - \lambda c, \quad (1)$$

where α denotes the constant dispersivity [m], \mathbf{u} the uniform vector-valued pore velocity [m/s] and $\lambda \geq 0$ the degradation [1/s]. Therefore, the first term on the right-hand side of (1) represents the diffusion and the second the convection term whereas the last term corresponds to the sink within the domain. Moreover, without limiting the generality, the point-source shall be located in the origin $(0,0) \in \mathbb{R}^2$ for further consideration. Similarly, it can be assumed that the pollution only propagates in x -direction, i.e. $\mathbf{u} = (u, 0)$ which can be achieved by affine transformation.

In the course of this comparison the transport equation (1) shall be solved numerically by the application of a finite difference method (FDM) and, a possibly more intuitive approach, the random walk (RW) method.

1.1 Task A: Unaffected pollution spread

The first task consists of the simulation of the pollution spread associated with the assumptions as described above. In this particular case, an analytical approximation can be stated: By assuming a steady source of pollutant on an infinite area where no sink exists, i.e. degradation $\lambda = 0$, the analytical solution of (1) can be approximated through

$$c(x, y, t) = \frac{c_0}{4\sqrt{\pi\alpha r}} e^{(x-r)/(2\alpha)} \operatorname{erfc}\left(\frac{|\mathbf{u}|t}{\sqrt{2\alpha|\mathbf{u}|t}}\right) \quad (2)$$

with the definitions

$$c_0 := \frac{M}{h n_e |\mathbf{u}|}, \quad r := \sqrt{x^2 + y^2},$$

and the (complementary) error functions

$$\operatorname{erfc}(\phi) = 1 - \operatorname{erf}(\phi)$$

according to [1].

The associated parameters M, h, n_e represent the input rate of pollutant mass, the thickness of the saturated flow and the effective porous volume respectively.

The computed results of both the FDM and RW based on the parameters of Table 1 shall be compared among themselves and with the approximated solution (2) at $t = 50$ and $t = 150$ days.

Variable	Description	Value
\mathbf{u}	Pore velocity in x -direction	10^{-5}m
α	Dispersivity	0.05m
λ	Degradation	0
M	Input rate of pollutant mass	0.002g/s
h	Thickness of saturated flow	10m
n_e	Effective porous volume	0.25

Table 1: Notation and description of used parameters.

1.2 Task B: Pollution reduction by facilities

In this task the impact of treatment facilities on the pollution shall be investigated. Therefore, it is assumed that a direct pollution reduction at the pollution source is not possible but treatment facilities can be installed at certain locations in order to reduce the pollution locally. In reality, this might be achieved by wells with chemical substances, pumps blowing in oxygen etc.

In order to reduce the pollution two plants of the treatment facilities are located at $(40\text{m}, \pm 5\text{m})$. The actual reduction of the pollution is modelled with the degradation parameter λ : Within a circle neighbourhood of 5m around each plant the degradation is set to $\lambda = \lambda_{\text{on}} := 10^{-6} \ln(10) 1/\text{s}$ which corresponds to a decrease in pollution concentration of 10% each $\delta t = 10^6\text{s}$ based on the assumed exponential pollution sink due to (1), i.e. $e^{-\lambda \delta t} = 0.1$.

The algorithms are supposed to be applied to the asymptotic solution obtained by task A. The computed results of both the FDM and RW shall be compared with task A at different locations after $t = 100$ days of active pollution reduction.

1.3 Task C: Controlled pollution reduction

Task C aims to model the scenario in which a reduction of operational costs is sought while maintaining a low pollution level is still desired. The setting for the comparison is equal to task B, but as opposed to $\lambda = \lambda_{\text{on}}$ permanently, the following strategy is applied instead: The degradation λ equals 0 from Monday to Friday between 8am and 8pm. Apart from these periods the degradation λ corresponds to $\lambda_{\text{on}} = 10^{-6} \ln(10) 1/\text{s}$ at the respective areas around the facilities. The results of both the FDM and RW shall be discussed at $(x, y) = (50\text{m}, 0)$ for $0 \leq t \leq 150$ days. In fig. 1 the situation is depicted for all tasks. The next chapters introduce the computational approaches for solving (1): The FDM and RW whereas both are implemented in Matlab.

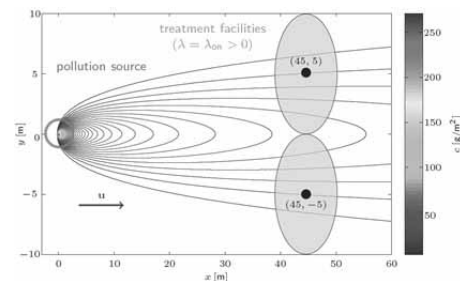


Figure 1: Pollution concentration obtained by (2) after $t = 150$ days with parameters of table 1 (task A). The green regions represent the 5m-circle neighbourhood of the treatment plants at $(40\text{m}, \pm 5\text{m})$ (task B and C).

2 Finite Difference Method

Mesh grid. By assuming equal steps h in x - and y -direction the mesh of the regarded domain shall be given by the nodes $(x_i, y_j) \in \mathbb{R}^2$. Furthermore, the approximation of the pollution concentration $c(x_i, y_j)$ at the nodes $(x_i, y_j) \in \mathbb{R}^2$ shall be denoted by $c_{i,j}$, i.e. $c_{i,j} \approx c(x_i, y_j)$. Thus, the inner nodes are described by (1) whereas for the nodes located at the boundary of the domain one may either set reasonable boundary conditions (b.c.) or assume the domain to be sufficiently large and then impose zero b.c. In this comparison the latter was chosen. Hence, for the comparison, simply the domain of interest is plotted whereas a larger domain was computed. The mesh grid was chosen to be $\{(x_i, y_j) : -10 \leq x_i \leq 100, -20 \leq y_j \leq 20\}$ whereby step size $h = 1/4\text{m}$ for the computation of all tasks. In the following, the discretization techniques of the involved terms in (1) are regarded separately.

Diffusion term. Given that both the steps in x and y are equal to h the second order discretization of the Laplace operator ∇^2 by means of a five-point stencil reads

$\nabla^2 c_{i,j} = (c_{i+1,j} + c_{i-1,j} - 4c_{i,j} + c_{i,j+1} + c_{i,j-1})/h^2$ for inner domain nodes. By using a lexicographical order for the indices and bearing in mind the zero b.c. the five-point can be represented as block tridiagonal matrices which were implemented as sparse matrices.

Convection term. Since $\mathbf{u} = (u, 0)$ it is reasonable to use a backward difference for the discretization of the gradient operator ∇ . Thus, it holds that

$$\mathbf{u} \cdot \nabla c_{i,j} = \left(u \cdot \frac{\partial c_{i,j}}{\partial x} \right) \approx u \cdot \frac{(c_{i,j} - c_{i-1,j})}{h}.$$

Again, the resulting block tridiagonal matrix was stored in sparse format in Matlab.

Time derivative. The remaining time derivative in (1) was implemented by means of an explicit Euler with time step $\Delta t = 2$ hours.

Evolution. The initial concentration was set to zero for all nodes and the concentration at the origin $(0,0)$ got augmented by $M\Delta t/h^2$ each time step Δt .

3 Random Walk

Modelling. The second method, the random walk, may be regarded as a more intuitive approach: Instead of solving the PDE (1) directly, transition probabilities are inferred which model the convection and diffusion behaviour of pollution *particles*. More precisely, the pollutant is modelled by means of a finite number of particles which execute a *deterministic convective* and a *probabilistic dissipative* movement: With (p_x^n, p_y^n) denoting the coordinates of one single particle at time $t = n\Delta t, n \in \mathbb{N}_0$, the particle movement is defined as

$$\begin{cases} p_x^{n+1} = p_x^n + \sqrt{2au\Delta t}Z_x + u\Delta t \\ p_y^{n+1} = p_y^n + \sqrt{2au\Delta t}Z_y \end{cases} \quad (4)$$

for one time step Δt whereby Z_x and Z_y represent standard, normally-distributed random variables. For the modelling each particle corresponds to an appropriate amount of pollution mass which depends on the step size and pollution source. Thus, there is no need for neither a mesh grid nor for collision rules. This type of approach has already been modelled in [2]. However, the procedure presented in here follows the explanations in [3] and therefore is defined slightly differently.

Pollution concentration. Even though no mesh grid is necessary for the computation, the mesh associated with the FDM is used in order to compare both methods. Each node is then assigned the pollution concentration given by the mass determined by the amount of particles located within an ε -neighbourhood divided by its area $\varepsilon^2\pi$. For task B and C the pollution reduction is modelled by particle weights ω : If a particle entered the scope of any treatment plant within Δt , it is set $\omega = e^{-\lambda\Delta t}$ whereby $\omega = 1$ at $t = 0$. The pollution reduction then corresponds to a reduced weight of the particle. In further consequence, the pollution concentration at each node can be obtained by considering the weights of each particle.

Evolution. It is assumed that additional 100 particles enter at the origin $(0,0)$ each time step $\Delta t = 2$ hours whereby the pollutant mass per particle is set to $M\Delta t/100$. The radius for the pollution concentration computation corresponds to $\varepsilon = 0.5\text{m}$.

4 Results

Task A: Unaffected pollution spread.

In Figure 2 the pollution concentrations according to both numerical approaches and the approximated solution (2) after $t = 50$ days are illustrated.

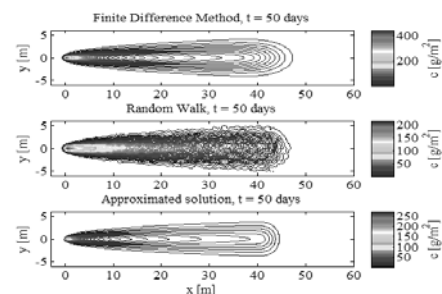


Figure 2: Task A: Pollution after 50 days for all methods

It can be witnessed that all results are qualitatively similar. However, especially at the vicinity of the pollution source the predicted concentrations differ which can also be observed in Figure 3. Moreover, FDM and RW agree quite well beyond approximately $x \geq 5\text{m}$. Nevertheless, the computed results of FDM and RW depend crucially on their parametrization, i.e. the choice of input rate ($M\Delta t/h^2$ at FDM, $M\Delta t/100$ at RW) and ε for the ε -neighbourhood (RW). Therefore, other values might yield a better alignment among all methods. For computational time, RW is more advantageous in general.

Task B: Pollution reduction by facilities.

The figures 4 and 5 show the impact of the pollution reduction facilities. At $x = 30\text{m}$ virtually no pollution reduction is recognized for both methods whereas their effect becomes the more manifest the higher the distances are. At $x = 50\text{m}$ the concentration has already dropped by more than a half compared to task A.

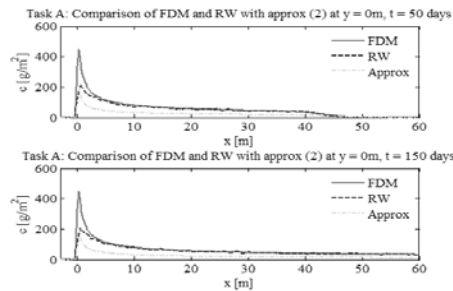


Figure 3: Task A: Pollution after 50 and 150 days at $y = 0\text{m}$.

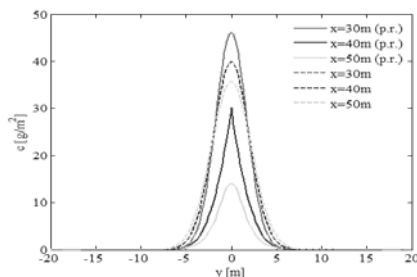


Figure 4: Task B – FDM: Pollution after 100 days at 30m, 40m and 50m with and without pollution reduction facilities.

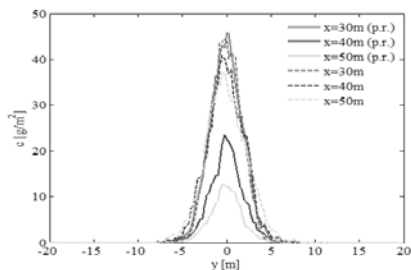


Figure 5: Task B – RW: Pollution after 100 days at 30m, 40m and 50m with and without pollution reduction facilities.

Task C: Controlled pollution reduction.

With respect to the controlled pollution reduction (fig 6 and 7) it can be witnessed that the pollution decreases steadily for both the FDM and RW until it remains small but fluctuates around 20g/m^2 . As opposed to the case of using a permanent pollution reduction according to task B (indicated by blue circles at some time points) the pollution concentration is slightly higher. However, a still substantial decrease is achieved and the benefit in cost savings may outweigh the higher pollution level.

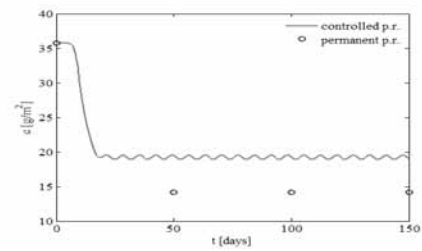


Figure 6: Task C – FDM: Comparison of pollution spread at $(50\text{m}, 0\text{m})$ for permanent and controlled pollution reduction.

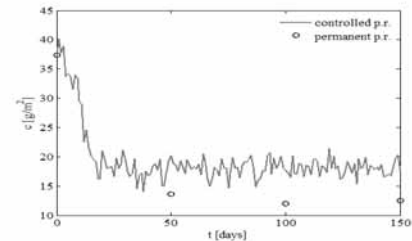


Figure 7: Task C – RW: Comparison of pollution spread at $(50\text{m}, 0\text{m})$ for permanent and controlled pollution reduction.

5 Conclusion

Both the FDM and RW yielded qualitatively comparable results. However, their actual figures depend considerably on the implementation of the input pollution rate at the origin. Hence, parameter studies could be necessary in order to find the right parametrization according to a particular problem in reality.

Model sources

Finite Difference Method and Random Walk Method are directly programmed in MATLAB. All MATLAB m-files and a short file documentation can be downloaded (zip format) by EUROSIM societies' members from SNE website, or are available from the author.

References

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