'Pollution in Groundwater Flow' – ARGESIM Benchmark C19R with Spatially Distributed Modelling

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The ARGESIM Benckmark C19R 'Pollution in Groundwater Flow' is based on a case study: in a homogeneous ground water body a singular pollution source contaminates the ground water stream; for decontamination, downstream two facilities are set up, which should reduce the contamination. Basis for modelling is the two-dimensional transport equation with degradation term for the pollution concentration, an analytical approximation for the solution in case of homogeneous flow, and an analytical approximation for the steady state. The benchmark first investigates the spread of pollution without counteraction, comparing numerical and analytical solutions. The more complex tasks of this benchmark deal with modelling and implementation of the facilities for decontamination and with calculating simulation results for continuous or schedule-controlled action of the facilities. The benchmark addresses quite different modelling approaches and solution techniques, from classical discretisation methods via FEM to alternatives techniques like cellular automata, Monte-Carlo methods and Random Walk.

Introduction

Since many years the demand for pure water is increasing, as well for human consumption as well as an ingredient in industrial processes. In many regions, the surface water available does not suffice, so more and more ground water has to be used. Exploring existing ground water bodies uncovers unfortunately many polluted areas, sometimes with unknown pollutant sources. In this exploration, data can only be gathered via wells, which is expensive and sometimes not possible. Therefore, modelling and simulation of a polluted groundwater body can help in various cases: determination of the pollution plume, localisation of the pollution source, planning of facilities for decrease of pollution, etc.

This benchmark is based on the following case study: in a homogeneous ground water body, flowing in x - direction, a singular pollution source contaminates the ground water stream. As the source is not known or situated in an inaccessible area, the groundwater must be decontaminated somewhere else in flow direction.

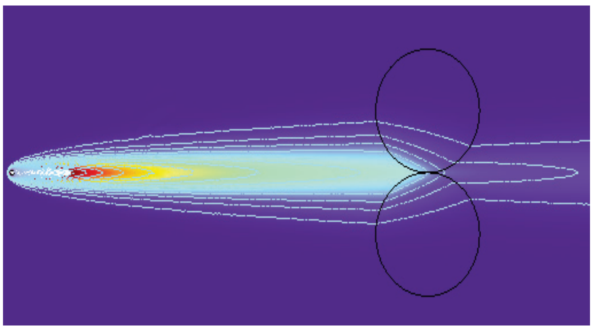

Figure 1: Polluted flow and effect of treatment facilities (FEM simulation).

A possible solution is to set up two treatment facilities – for example air spargers, which force oxidisation – symmetrically to estimated maximal flow in x - direction. Figure 1 shows this situation, whereby the polluting source and the effect of the facilities can be seen.

Basis for modelling of the groundwater flow is the transport equation, describing the pollution concentration, a PDE with constant or state-dependent parameters and more or less complex boundary conditions. Of importance are furthermore analytical approximations for the pollution concentration in the homogeneous case, which may be compared with numerically calculated solutions. For modelling and simulating decontamination by degredation terms in the PDE, investigation start in an appropriate approximation for the steady state solution.

In principle, quite different modelling approaches and solution techniques can be applied, from classical discretisation methods via FEM to alternatives techniques like cellular automata, Monte-Carlo methods and Random Walk. In simple cases also approximating analytical solutions may exist. But in any case, or any chosen approach, there must be the possibility to embed analytical approximations, and to model or calculate a steady state solution. In reality, the choice of a modelling method or solution technique, may also depend on the data available, and on the aim of the simulation.

This comparison investigates different modelling methods and solution techniques with increasing degree of difficulty. First the spread of the pollution is without any counteraction is considered, whereby numerical solutions are to be compared with the analytical approximation.

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In the following the pollution spread influenced by the counteraction with two treatment facilities investigated; for this inhomogeneous flow, boundary conditions for subregions must be noticed, and as initial condition a steady state must be found. And finally, the action of the treatment facilities should be controlled by a time schedule.

1 PDE Model for Pollution Concentration

Basis for modelling is the transport equation, describing the concentration $c(t, x, y)$ of a pollutant in the saturated zone of a homogeneous two-dimensional ground water body with respect to both convection and dispersion. A simplified version of the transport equation is:

$$\frac{\partial c}{\partial t} + \frac{u_x}{R} \cdot \frac{\partial c}{\partial x} + \frac{u_y}{R} \cdot \frac{\partial c}{\partial y} = \\ = \frac{\alpha_L \cdot |\vec{u}|}{R} \cdot \frac{\partial^2 c}{\partial^2 x} + \frac{\alpha_T \cdot |\vec{u}|}{R} \cdot \frac{\partial^2 c}{\partial^2 y} - \lambda \cdot c$$

which lacks the general terms for sources and sinks, as they will be kept simple in this example, but includes a degredation term which will be needed.

Table 1 shows parameter values being typical for the slow flows under investigation. Note that the porous velocity u_x is equal to about 1.7 meters by day, which is quite fast for groundwater but was chosen to ease modelling and simulation. It should also be mentioned that the porous velocity is only the average speed of water and the contained pollutant, averaging over every possible path in the porous strata forming the aquifer.

Description	Name	Value
pore velocity	$\vec{u} = \begin{pmatrix} u_x \\ u_y \end{pmatrix}$	$\vec{u} = \begin{pmatrix} 10^{-5} \\ 0 \end{pmatrix}$ m/s
dispersivity	$\alpha_T = \alpha_L$	0.05 m
retardation factor	R	1
degradation	λ	0 1/s
thickness of the saturated flow	m	10 m
effective porous volume	n_e	0.25
input rate of pollutant mass	M	2 mg/s

Table 1: Parameter values for pollution spread.

The effective porous volume n_e is the fraction of the water bearing stratum (aquifer) which is used by the groundwater flow, and is derived with experiments. In this comparison 1 m^3 of material with an effective porous volume $n_e = 0.25$ can contain up to 250 litres of water. This maximum is actually reached in the saturated zone, which is the zone considered in this investigation. The $h = 10$ meters of soil therefore represent 2.5 meters of water.

2 Analytical Approximation in Steady State

Assuming a steady source of pollutant M in (0, 0) on an infinite area allows to derive an approximating solution for the concentration $c(t, x, y)$ for the parameters given in Table 1 by a product of exponential function and complimentary error function:

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

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

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

This approximation is a slightly simplified form, taking into account the isotrophy of the aquifer and the simple form of the ground water flow. It also incorporates the assumption that the concentration does not differ in z - direction, which is accomplished by the term $m{\cdot}n_e$ in the denominator of the formula for c_0, just dividing the pollution by the 2.5 meters of water. Especially important is the retardation factor 1, which stands for no retardation – the pollutant does neither react nor compound with the soil, and is instantly transported.

By means of the analytical approximation, e. g. in case of homogeneous spread of the pollution, the ‘pollution wave’ can be calculated with reasonable accuracy (Figure 2, c(x, y, t) for $t = 40$ days, $t = 60$ days, $t = 80$ days).

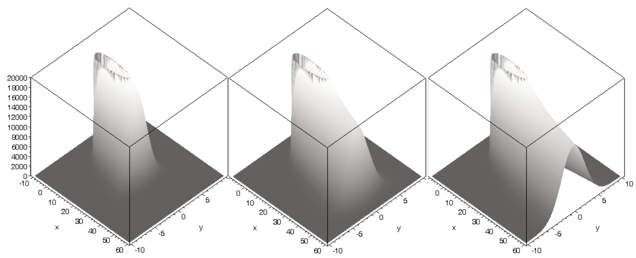

Figure 2: Evolution of pollution wave for $t = 40$ days, $t = 60$ days, and $t = 80$ days.

3 Experiments - Tasks

The classical ARGESIM Comparisons require three tasks to be performed with the defined dynamic system, mostly addressing investigations and analysis in the time domain; furthermore information on the simulator used and a short description of the model implementation should be given - all to be presented within one page SNE. The new or revised ARGESIM Benchmarks extend the three tasks - Task **A**, Task **B**, Task **C** - and the simulator description - Task **S**imulator - by requesting a detailed description of the model implementation, whereby also different modelling approaches may be presented - Task **M**odelling, and by a short resume of the benchmark solution - Task **R**esume, trying also a classification of the approach. For presentation of all tasks two pages SNE may be used (task **M**odelling min. ¾ page SNE.) Furthermore, model source files should be sent in. More details at WWW.ARGESIM.ORG, menu *SNE*.

Modelling. This benchmark can be tackled by very different approaches, from FEM via classical PDE discretisations to alternative methods like Cellular Automata and Random Walk. So we ask for a presentation of the approach used - in case of alternative approaches the 'mapping' of the PDE onto the chosen algorithm should be sketched. In case of graphical modelling tools, please provide snapshot from the modelling procedure. Furthermore, the model implementation needs significant model extensions especially for Task **B** and Task **C**, which should also be documented.

A - Task: Simulation of Pollution Spread. Under simplified conditions, the concentration of pollution spreads from the source into x - direction looks like a plume (Figure 3). There exist a lot of approaches and numerical techniques for solving the transport equation. Aim of this task is to compare a numerical solution based on any technique with the approximate analytical solution given before for the homogeneous case under investigation.

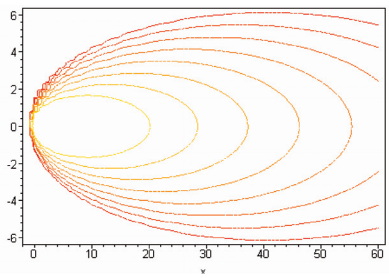

Figure 3: Pollution - isolines, plum-like spread.

Have in mind that the analytical solution is derived by using an infinite plane, and accommodate this in your model. When using the Finite Element Method or Finite Differences, you will almost certainly do this by using a flux boundary conditions of appropriate types.

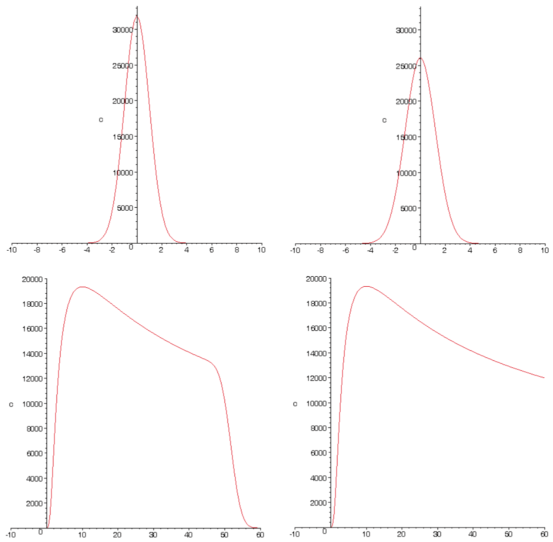

Figure 4: Pollution concentration, x - and y - sections.

During the direction of flow, the mass flow will be mostly convection driven at the right boundary, diffusion driven on the lower and upper boundary, and non-existing at the left boundary if chosen not too close to the source of the pollution, as upstream spread is only driven by dispersion.

Sections of any kind give information on the pollution spread. Figure 4 shows sections for x and y ; Figure 5 is the so-called break-through curve, showing the pollution wave passing a certain position.

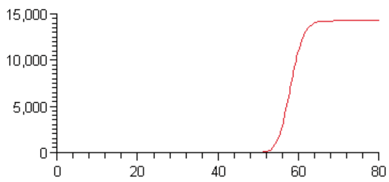

Figure 5: Pollution break-trough curve for postion ($x = 0,\ y = 40$).

For comparing numerical and analytical simulations, a rectangular area with $-10 \le x \le 60$, $-20 \le y \le 20$, is chosen, with constant pollution source $M = 2.0$ mg/s in place $(0, 0)$ - other parameters see Table 1, with observation period of 150 days. Results should be compared with the analytical approximation at the line $(50, y)$ at $t = 50$, $t = 100$, and $t = 150$ days (absolute values and differences).

B - Task: Pollution Reduction by Facilities. Main goal is to reduce or to eliminate the pollution. As the pollution source cannot be influenced directly, facilities can be set at certain locations reducing the pollution locally (wells with chemical substances, pumps blowing in oxygen for precipitation, etc.). In the surrounding of such facilities locally elimination of the pollution takes place, reflected by an increase of the degradation parameter in the transport equation in a neighbourhood of the location.

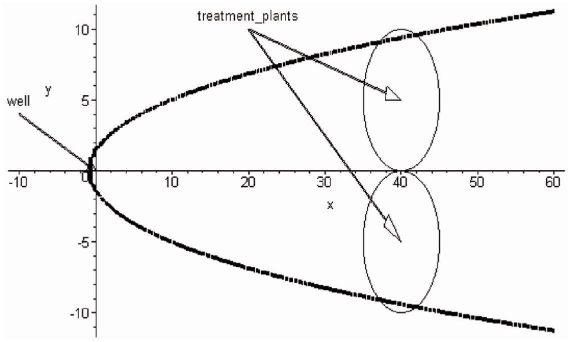

Figure 6: Boundary of pollution (thick line), influence areas of plants (thin circle lines).

The task is now, to investigate the influence of a facility with two plants. In order to get reasonable results, investigations should start from a steady state solution $c(x, y, \infty)$. With K_0 being the modified Bessel function of second kind, and with c_0 and r as before, the steady state solution is approximately given by

$$c(x,y,\infty) = \frac{c_0}{2\pi\alpha} e^{\frac{x}{2\alpha}} K_0\left(\frac{r}{2\alpha}\right),\ K_0 = \int_0^\infty \frac{\cos xt}{\sqrt{t^2+1}} dt$$

From engineering viewpoint, this formula is a very good approximation for the steady state solution. For arguments $(r/2\alpha) > 1$ the approximation shows an error of about 10 %, which drops down to less than 1 % for arguments $(r/2\alpha) > 10$.

The facility consists of two plants situated at (40, 5) and (40, -5). The effect of the plants on the contamination is modelled by a degredation parameter λ being non zero in a surrounding of the plants. A reasonable choice is a value $\lambda = -10^{-6} \cdot \ln 10$ in a circle neighbourhood of each plant with a radius of $d/2 = 5$ m centred on the coordinates of each plant.

Figure 6 shows this scenario: place and action radius of the plants allow an degredation across the full width of contamination. The degradation lets drop down the pollutant concentration c to 10 % for a given control volume spending exactly 10^6 seconds in one of those areas. 10^6 seconds is that time span, the control volume would need to cross the circles right across the diameter d of 10 meters, the average remaining concentration will be much higher then that 10 % .

The task is now, to model this scenario appropriately, starting from the given steady state solution (approximation) and to investigate the degredation of pollution in time and space. We ask for documenting the implementation or numerical calculation of the steady state solution, and for display of simulation results.

Results for pollution and degradation should be documented as plot of the lines $(30, y)$, $(40, y)$, and $(50, y)$, $20 \le y \le 20$, for $t = 100$ days.

C- Task: Controlled Pollution Reduction. To minimize costs for operating the plants and to allow for maintenance, the hours of operation must be limited. A reasonable strategy lets the plants operate only during night and at weekend, so that maintenance can be done at regular working hours, and so that the cheaper electric energy during the night hours can be used.

This strategy can be modelled by a periodical change of the degradation parameter λ from $\lambda = -10^{-6} \cdot \ln 10$ (plants on) to $\lambda = 0$ (plants off).

Task is now, to model this strategy appropriately (please give implementation details) and to simulate the system starting from the steady state solution with the following strategy:

- plants are active Monday to Friday from 0 to 8am and from 8pm to 12 pm,
- plants are active weekends around the clock, and
- plants are switched off else

As result, plots against time are now appropriate: plot the concentration at (50, 0), i.e. $c(50, 0, t)$ for $0 \le t \le 150$ (days) for switched operation given above, together with concentration for continuous operation (results from Task **B**).

References

[1] W. Kinzelbach: *Groundwater Modelling - An Introduction with Sample Programs in BASIC.* Elsevier Science Publ., 1986.

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