Flowpath-simulation in potential hazard studies for contaminants in groundwater

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Abstract

Studies on the potential hazard of a contamination often use flowpath simulation as a technique applied in combination with a flow model. Some numerical aspects and alternatives are presented and evaluated. The time-integrated approach turns out to be the method of choice. For the mentioned purpose the application of particle tracking should be used with care, because it is not conservative. The danger may be underestimated in areas transverse from the pathlines downstream from a contaminated site.

1 Introduction

In hydro-engineering practice it has become a widespread technique to use particle tracking as post-processing tool to a flow model. The visualisation of the flow pattern by pathlines resp. streamlines is used for different purposes. Reilly & Pollock [10,11] study areas contributing recharge to wells and their seasonal and long-term changes. Delineation of contributing areas is the problem tackled by Barlow [1] with the very technique. Within the international HYDROCOIN [6] project tracking algorithms have been studied for safety analyses for nuclear waste repositories. Johnson, Ravi & Rumery [7] estimate solute concentrations using a pathline counting method.

In this paper flowpath simulations are studied that are applied as a tool to estimate the potential hazard caused by contaminations in groundwater. Using the method flowpaths, here used synonymous with pathlines, are traced downstream from a contaminated site or upstream from a vulnerable region. In that way regions of influence can be determined. They provide informations to make a decision about the danger resulting from the transport of pollutants. Mostly the criterion is quite simple: there is no danger if one out of the two following situations is given

- there is no well within the region of influence from a contaminated site
- there is no contamination within the regions of influence for the wells
There are some advantages, which may explain the popularity of the method and which makes it the method of choice in comparison to transport modeling techniques. The main advantage is that there are no additional hydrogeological, physical or chemical parameters needed. Thus all those difficulties connected with the determination of parameters becomes obsolete. No need for calibration runs with a numerical model on a computer in order to determine aquifer dispersivities. No need for tracer experiments. No need for column or batch experiments in the laboratory in order to get Langmuir- or Freundlich-sorption isotherms (the determination of linear sorption parameters may be a reasonable extension of the method, as will be lined out below).

Nevertheless it will be shown that, what seems the advantage of the method, in fact is the main disadvantage as well. In cases where the neglected processes are relevant, the flowpath technique may not be able to provide good predictions. The danger resulting from transport of contaminants may be overestimated in parts of the environment and underestimated in others.

2 Numerical methods

2.1 General description

In order to simulate advective transport in a flow field various 'particle tracking' algorithms can be used. Starting at user-defined origin the path of a particle can be traced forward until the boundary of the region or a sink is reached. Tracing is likewise possible backward in time: from start the path is traced until boundary or a source are reached.

Codes are different in the form, in which the flow field needs to be given. Bear & Verruijt [2] present cases, in which velocities are given by explicit analytical expressions. Making a choice for the timestep $\Delta t$ (positive for tracing in future, negative for tracing in the past) the path is traced by using the Euler-method:

$$\Delta x = u_x \Delta t \quad \Delta y = u_y \Delta t \quad \Delta z = u_z \Delta t$$

or:

$$\mathbf{r} = \mathbf{r}_0 + \Delta t \cdot \mathbf{u}(\mathbf{r}_0, t_0)$$

Velocity components $u_x$, $u_y$ and $u_z$ are estimated using the location, where the particle stayed at time $t$ at the beginning of the timestep. This procedure is only applicable, if velocities are known at each location in the region. This is not possible, if the flow field comes out of a numerical model.

Tracking-algorithms, which can be applied in connection with a flow model need to take into account the discrete form of the velocity field. Values are given at certain locations only: at block-medium points, at volume boundaries or element edges of a discrete grid.

Using the code STLINE (Ward & Harrover & Vincent & Lester [13]) it is assumed, that velocities (given in the block centers of a rectangular grid) change linearly along the space in between. The distances $(\Delta x, \Delta y, \Delta z)$ covered in a timeperiod $\Delta t$ can be calculated according to (1) or (2), if velocity components are taken from the nearest block centers. An example: in x-
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The linear formula \( u_x = a + bx \) is used, where \( x \) represents the local variable in the block. The coefficients are then given by:

\[
a = u_{x1} \quad \quad b = \frac{(u_{x2} - u_{x1})}{\Delta x}
\]

\((u_{x1} \text{ resp. } u_{x2} \text{ denote velocity components at block centers})\). Then holds:

\[
\Delta x = \frac{(a + bx)\Delta t}{1 - b\Delta t / 2}
\]

Proceeding like this for all coordinate directions the location of the particle at the end of the time period can be determined. A problem with the method is, that the final location should not be outside the block from which the velocities have been taken. STLINE overcomes the problem partially by using smaller timesteps. Nevertheless, this does not prevent the method, to calculate a final location of the block another time. On the other hand, a repeated use of the procedure reduces the distance of overshooting and thus the errors resulting from a false velocity estimation.

Some other aspects should be mentioned briefly. Velocity fields determined by linear interpolation as described above, fulfill the usual differential equation for groundwater flow. The field is rotation free, for \( u_x \) is a function of \( x \) and \( u_y \) is a function of \( y \). But divergence may not necessarily vanish in steady state. Treating both directions as described in the 2-dimensional case the following is obtained:

\[
\text{div } \mathbf{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = \frac{u_{x2} - u_{x1}}{\Delta x} + \frac{u_{y2} - u_{y1}}{\Delta y} = \frac{1}{\phi S \Delta x \Delta y} (v_{x2} \Delta y - v_{x1} \Delta y + v_{y2} \Delta x - v_{y1} \Delta x) = 0
\]

In equation (5) particle velocities \((u)\) are related to darcy-velocities \((v)\), porosities \((\phi)\) and saturations \((S)\). Finite volume discretisations generally fulfill the last equation in the block interior, because they are based on the finite formulation given in the brackets. At block edges there may be jumps of \( u_x \) resp. \( u_y \), when there are different parameter values for \( \phi S \) in the adjacent blocks. Furthermore, at edges with constant \( x \) the \( u_x \)-component and at edges with constant \( y \) the \( u_y \)-component may have discontinuities themselves. In order to avoid this inconsistency Goode [4] recommends bilinear interpolation. Nevertheless, these have the disadvantage, that they do not fulfill the differential equation in the interior of the blocks.

For the numerical integration in time approaches of higher order can be used, replacing the simple Euler method given in equation (1). Methods of Runge-Kutta type are often described in publications. Sauter & Beusen [12] apply the 2. order Heun-method. In their algorithm the Euler-method is used to determine a first approximation for the particle location \( r \) at the end of the timestep. In a second step the velocity at position \( r \) is taken to determine the second and final location:
There are various other Runge-Kutta type approaches, which can be used alternatively. I want to mention just one more, which starts with an Euler step with timestep $\Delta t/2$ gemacht. The position from that calculation is then used to determine an improved velocity approximation for the second step starting again at the initial location:

$$\tilde{r} = r_0 + \frac{\Delta t}{2} \cdot u(r_0)$$

$$r = r_0 + \Delta t \cdot u(\tilde{r})$$

All these approaches can be generalised for 'particle tracking' in transient flow fields. With higher order schemes the problems, which occur when a block boundary is approached, cannot be solved. This can be achieved by a time-integration, which is based on the analytical solution, that exists under certain conditions. $\Delta t$ loses it’s characteristic as a user-defined control parameter for the accuracy of the solution.

2.2 Time-integrated approach

As mentioned above the time-stepping approach leads to problems when block resp. element boundaries are passed in the considered timeperiod $\Delta t$. In order to overcome this problem, a time-integration approach can be used. The method is described as implemented in the FASTpath code, which was developed by the author (Holzbecher [5]). The program is designed as a post-processor for steady-state flow fields, which are calculated by block-centered finite difference or finite volume models. Nevertheless the method can be applied to general cases.

In FASTpath the problem is avoided by giving a different role to timesteps. $\Delta t$ is no longer a user-defined guess to influence the lengths of discrete steps in the tracking procedure. By time-integration an analytical solution is determined, from which the exact locations can be calculated where a flowpath enters and leaves a block. The method starting at one origin then connects block-exit points.

![Figure 1: Distances and denotations in a rectangular grid block](image-url)
The FASTpath algorithm is based on the assumption, that velocity components are given normal to the block edges. As in other codes the method is based on the assumption, that within a block velocities change linearly. The time which the particle takes to move from one block edge to the other can be determined analytically.

If $u_{x1}$ resp. $u_{x2}$ denote velocity components at block edges, $a$ and $b$ from equation (3) can be used to interpolate $u$ for the block interior. The traveltime for a particle between coordinates $x_0$ and $x$ can be calculated by:

$$
\Delta t_x = \int_0^x dt = \int_{x_0}^x ds = \int_{x_0}^x \frac{ds}{a + bx} = \frac{1}{b} \ln(a + bx) \bigg|_{x_0}^x
$$

$$
= \frac{1}{b} \left[ \ln(a + bx) - \ln(a + bx_0) \right] = \frac{1}{b} \ln \left( \frac{a + bx}{a + bx_0} \right)
$$

In figure 1 the situation is shown for $x_0$ as the value of the local variable at the block entrance point. The formula holds for all $x$-values that fall inside the block. Especially the maximum traveltime within the block if the maximum value for $x$ is taken ($\Delta x - x_0$ if flow is in positive $x$-direction, 0 if flow is in negative $x$-direction):

$$
\Delta t_x^{\text{max}} = \begin{cases} 
\frac{1}{b} \ln \left( \frac{a + b(\Delta x - x_0)}{a + bx_0} \right) & \text{for positive velocity} \\
\frac{1}{b} \ln \left( \frac{a}{a + bx_0} \right) & \text{for negative velocity}
\end{cases}
$$

The traveltime from equation is the real one, if the flowpath reaches one of both edges $x=0$ or $x=\Delta x$. In a more dimensional case there are other possibilities. Thus in the same way the other coordinate axes have to be treated and the actual traveltime in the block (in 3-dimensional flow) is the minimum of the ones determined for the directions:

$$
\Delta t = \min \left\{ \Delta t_x^{\text{max}}, \Delta t_y^{\text{max}}, \Delta t_z^{\text{max}} \right\}
$$

After the time period $\Delta t$ the flowpath reaches the boundary of the block. Using $\Delta t$ the exact location of the block-exit-point can be calculated easily using equation (2). Solving for the local variable $x$ provides:

$$
x = \frac{1}{b} \left[ (a + bx_0) \exp(-b\Delta t) - a \right]
$$

Similar equations hold for the other coordinate directions. The transformations leading to equation (11) are valid, if $b \neq 0$ and if $a$ and $x_0$ do not vanish simultaneously. If $b=0$ then there is a constant velocity in $x$-direction and the maximum traveltime results from the simple formula:
\[ \Delta t_x = \frac{1}{a} (x - x_0) \quad (12) \]

If \( a=0 \) holds, then there a stagnation point at the concerning block edge. If with \( x_0=0 \) the block is reached at this edge, the particle does not move further into the block interior. In the algorithm the maximum traveltime can be formally set to the maximum machine constant (equivalent \( \infty \)) and the position is \( x=0 \).

Other exeptions have to be formulated for source- resp. sinkblocks. These are characterised by the fact that there are is outflow resp. inflow at all edges. Sinkblocks thus have no exit in forward particle tracking, sourceblocks have no entrance in backward tracking. Traveltimes within these blocks are highly speculative, because the very local nature of flow in the vicinity of infiltration resp. pumping wells is reduced to a mass balance relation, when a computer model for groundwater flow is used.

![Flowpath calculated with FASTPATH](image)

**Figure 2**: A flowpath as connection of entrance- resp. exit-points

An equivalent formulation of the algorithm implemented in the FASTpath code was published by Pollock [9]. A generalisation for non-rectangular grids can be found in Cordes & Kinzelbach [3].

The method has been described for steady state flow fields here. Nevertheless the extension to transient cases is straight-forward. It has additionally been taken into account, that there is a moment, when the current velocity field needs to be replaced by a new one. It is intended to improve the FASTpath code in that way.

### 3 Application

Flow fields can be visualised by particle tracking. In two-dimensional steady state cases the flow pattern can be presented in a single plot. Figure 3 shows the flow towards a pumping well, which is located on the boundary of the modelled area; i.e. only one half of a horizontal cross-section is considered. The other half can be obtained by symmetry. Approximately half of the water entering at the boundary on the right hand side reach the well (5 out of 10 pathlines are traced into the well).

Figure 4 shows the same system, where a second well with a lower pumping rate was installed in order to catch polluted fluid entering from the right hand side. The limited effect of the protection well is clearly visible in the
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Figure: only those pollutants are withdrawn, which are transported with the flow field from the the small area (A). Moreover the first well pumps water from the far side of the system: the upper 4 pathlines only reach and cross the outflow boundary on the left side. If the contaminated area extends into that region (B), the installation of the second well is even contraproductive: the quality of pumped water worsens.

Figure 3: Visualisation by flowpaths: flow towards a pumping well

Figure 4: Flow towards a pumping and a designed protection well

The example demonstrates the application of particle tracking. In order to determine, if water quality in a pumping well is worsened from a contaminated site, it needs to be recognized, if well and polluted area are combined by at least one pathline. Practically this is done by an interactive use of the flowpath software: startpoints for pathlines are specified by the user just on the basis of the visual impression from the flow graph.

Backward and forward tracing in principle are both useful to determine possible connections. In both cases regions of influence are of interest. The region of influence downstream from a contaminated zone is reached by advectively transported pollutants. For a single well or a well gallery the pumped water originates from the region of influence. In 2-dimensional horizontal flow tracking backward in time leads to catchment areas.

Particle tracking simulates advective transport as the only process. All other processes which influence the distribution of pollutants in the subsurface are neglected. In the remaining part of this section will be discussed, how the results from the flowpath technique as described above, can be judged in
relation to results from a common transport model, which considers other processes. Especially the question will be answered, if the method is conservative.

3.1 Neglection of longitudinal dispersion
Along the flowpath polluted fluids are subject to mixing processes as diffusion and longitudinal dispersion. Peak concentrations are reduced. On the other hand values increase in low concentrations regions. When the flowpath method is used as described above - by determination of influence regions - the method always leads to an overestimation of risk. In principle the technique is based on the conservative assumption, that there is no mixing along the pathline and thus concentrations are kept high. Nevertheless in real systems mixing always is a substantial process.

From the aspect of mixing along a pathline the use of the flowpath technique always leads to conservative results.

3.2 Neglection of transverse dispersion
In directions transverse to the flowpath mixing processes occur as well. Diffusion and transverse dispersion are responsible, that a plume of pollutants not only spreads in the direction of flow. Though these moments are neglected by using flowpath tracing as described above, the potential danger is underestimated in regions which are not hit by pathlines which pass a contaminated region.

From the aspect of mixing transverse to a pathline the use of the flowpath technique does not lead to conservative results.

3.3 Neglection of decay resp. degradation processes
If any decay or degradation are relevant processes the result is a decrease of pollutant concentrations relative to another component which is not degraded. The flowpath technique does not account for these processes and thus predicts a higher risk for decaying contaminants. If the pollutant reaches a vulnerable region, it may be mostly degraded. From the aspect of decay the use of the flowpath technique always leads to conservative results.

It is generally not possible to estimate peak maximum concentrations considering the traveltime along the flowpath. In real systems, mixing and decay interact in a way, which cannot easily be predicted, even if initial concentrations are known. A more specific statement can be made, when analytical solutions are studied - which is beyond the scope of this contribution. It is worth mentioning, that under certain conditions the decrease of maximum concentrations along a pathline can be estimated. If there is a single peak for the pollutant concentration as initial condition, the peak of the n-dimensional analytical solution declines with time according to (Kinzelbach [8]):

$$c(x,t) = \frac{\exp(-\lambda t)}{(\sqrt{t})^n}$$ (13)
Nevertheless in practical cases it is difficult to check if the conditions for the application of these formulae are fullfilled.

3.4 Considering linear sorption as retardation
If the interaction between fluid and porous medium concerning the concentrations of a component can be described by a constant linear isotherm, the description of the processes can be simplified by the introduction of a retardation factor. This does not change anything, if the decision about the potential hazard of a contaminated site is made following the above mentioned criterion. The condition depends on the connection of pathlines only and not on the timescale of the flow.

Retardation can be considered with the flowpath technique. It should be noted, that the problem of transverse mixing is less relevant for retardated contaminants, because the timescale for dispersion processes is reduced as well.

3.5 Neglection of non-linear sorption processes
It is not possible to do the same analysis as in the preceding section, if sorption acts obeying certain non-linear relationships, as the Langmuir- or the general Freundlich-isotherm. Retardation factors can be introduced in that case as well, but these are concentration dependent and thus change along the flowpath spatially and temporally. The resulting distribution patterns are thus more complicated.

The same holds for non-equilibrium sorption. It is beyond the scope of this paper to attempt a general statement concerning over- resp. underestimation by the flowpath technique for generalised sorption behaviour.

4 Conclusional remarks

The technique of flowpath simulation to study the potential hazard of contaminations should be applied with caution. The danger resulting from a pollution may be underestimated in parts of the environment, but overestimated in others. The modeler should keep in mind, that advection is the only transport process, which is visualized by flowpath tracing. Effects from dispersion, diffusion, decay and degradation cannot be taken into account. Linear equilibrium sorption can be considered, as long as it acts as a constant retardation. The movement of a concentration peak can thus be predicted but not the peak’s height.

Particle tracking combined with a decision based on pathline connections, is not a conservative method. Pollutants in real systems partially move transverse to flowpaths and there may increase concentrations above reasonable limits. To overcome this obstacle the criterion based on the connected pathlines could be altered. It could be required, that there is a certain distance between a pathline for polluted fluids and the catchment of a well. Nevertheless the quantification of that spacing can only be based on an estimation of transverse dispersivity.
References

6. HYDROCOIN - an international project for studying groundwater hydrology modelling strategies, OECD, Paris, level 3