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Heterogeneity influence on groundwater age

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SUMMARY

Groundwater age is considered as an important water property and can indicate its quality. Insufficient number of data and measurements in the subsurface has been mitigated by using direct simulation of groundwater age. Numerical model is developed using Lagrangian approach and random walk particle tracking method, where groundwater age is calculated as travel time of certain particles including the processes of advection and dispersion. For proposed method, flow calculation is the basic input; hence an upgrade has been done to existing software solution in order to get correct groundwater age simulations and continuous velocity fields. Synthetic examples were simulated for homogeneous, layered and for low and medium heterogeneous aquifer systems. For the heterogeneous aquifer system a stochastic analysis has been done using a Monte Carlo simulations. The results are given as groundwater age fields. An application is recognized in possibility to estimate the expected groundwater age at certain location of water intake. Therefore, calculated probability distributions may be used as decision support tool in order to estimate the level of aquifer's auto purification, or to apply certain level of water treatment before usage.

Key words: *groundwater age, Lagrangian approach, random walk particle tracking method, heterogeneity, Monte Carlo simulation, probability distributions of groundwater age.*

1. INTRODUCTION

Groundwater is commonly good source of quality drinking water due to less exposure to pollution than surface water and purification properties of soil. Close connected to quality of groundwater is groundwater age. Groundwater age is, by definition, time measured from entering of particle into soil system to specific location in groundwater system to time when it is sampled or theoretically observed in simulation of groundwater age.

The applications of groundwater age data are grouped into two categories; those that are general applications and those that are site-specic. Those data are used to evaluate the renewability and capacity of groundwater reservoirs, to estimate the groundwater capability of autopurification by porous media, to estimate groundwater recharge, to determine fracture and matrix properties and water velocities in fractured rock environments, to help study the trend of groundwater pollution, to identify past seawater level fluctuations, and to be used in many more hydrological applications such as mixing groundwater–surface water interaction, and seawater intrusion [1].

Most of the methods for calculating the age of groundwater used isotope, or radioactive tracers that are more or less reactive with the environment. But as such, tracers are not fully comparable with the water particles and can generate errors in groundwater age calculation. Goode [2] introduces age mass concept and directly solves new adopted transport equation using Eulerian approach and finally mean calculating groundwater age equation. Varni and Carrera [3] provided the moments of groudwater age. That solution enabled involvement of dispersion into the calculation process, which showed up to generate errors if ignored [4]. Though last decades scientists have indicated that the influence of heterogeneity and groundwater mixing due to hydrodynamic dispersion might produce uncertainty in environmental tracer-based age date results [3, 5-10], the magnitude of this effect is largely unknown. Interpretation of groundwater ages typically rests on assumptions of minimal mixing of different water ages in the water samples. The effects of three-dimensional, geologic heterogeneity on groundwater mixing and tracer concentrations, have been evaluated by Weissmann, Zhang, LaBolle and Fogg [11]; however without analysis of uncertainty around mean age. Recently, Wollfenden and Ginn [12] and Ginn, Haeri, Massoudieh abd Foglia [13] presented modelled groundwater age distributions as weel as usage of groundwater age in inverse and forward modelling.

This paper is motivated by Goode's idea of direct simulation of groundwater age but uses Lagrangian approach and particle tracking method similar as Rilley, Plummer Philips and Busenberg [7] in their advective model, with an extra part of using random walk particle method to include the dispersion in the process. After model is developed and calculations done for the comparable examples, we go step forward to introduce the impact of heterogeneity on final groundwater age results. Using Monte Carlo method to generate random fields of different hydraulic conductivity conditions, we calculated groundwater age layers for each simulation and applied stochastic analysis to produce probability density functions (PDFs) for groundwater age in chosen nodes of domain. Using calculated PDFs, probability estimation for groundwater age is given as direct application of proposed method. Same calculation has been done for lower and medium level of heterogeneity to show the impact. Groundwater age may be used as an indicator for water quality, considering purification and filter properties of aquifer that has been observed and/or simulated. Similar approach can be applied if we investigate possible pollution plume that may be transported with water and therefore estimate the probability of pollution occurrence at certain point, such as groundwater intakes.

2. METHODOLOGY

2.1 Lagrangian approach - particle tracking random walk method

Starting point of the approach is general equation for 2D transport with generally spatially variable velocity field and dispersion tensor depending on velocity as follows:

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}+D_{xy}\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}+D_{yx}\frac{\partial c}{\partial x}\right)-$$
$$-v_x\frac{\partial c}{\partial x}-v_y\frac{\partial c}{\partial y}=\frac{\partial c}{\partial t} \qquad (1)$$

where c (mass in unit volume [kg/m^3]) is substance concentration in groundwater driven by water flow conditions with v_x and v_y as water velocity components [m/s]. D_{xx}, D_{xy}, D_{yx} and D_{yy} are components of dispersion tensor where each of them is calculated by:

$$D_{H\,ij}=D_m\delta_{ij}+\alpha_T\left|v\right|\delta_{ij}+\left(\alpha_L-\alpha_T\right)\cdot\frac{v_iv_j}{\left|v\right|} \qquad (2)$$

where δ_{ij} is Kronecker's delta symbol, α_L [m] and α_T [m] are the local longitudinal and transverse dispersivities.

Transport can be modelled using Eulerian and Lagrangian approach. Depending on the application of specific numerical procedure certain numerical instability may occur. Numerical stability in the stationary system depends mostly on the choice of the size, and the number of elements in the use of finite element method. Criterion used for defining numerical stability is Peclet's number, and it has values from *100* to *1000* in underground, which makes Lagrangian approach more suitable as its stability is not affected by Peclet's number while Eulerian has lot of numerical instability for Peclet's number higher than *2*.

Lagrangian approach, used in this paper, is based on tracking particle from initial position and describing it trajectory over time and space. We use random walk particle tracking method (RWTP), where the particle tracking is used to describe the advection and random walk to describe dispersive movement.

When using the aforementioned method weight carrying virtual particle is monitored in time and space, in a way that advection is defined by velocity field (the result of flow calculation), and dispersion is described by statistical approach [14]. After each time step within which the process is observed, the concentration is calculated by summing up all the particles in each element of the control volume. This paper uses described method without calculating any concentration, but rather applying expressions for defining water particles positions:

$$\begin{aligned}
&x_p(t+dt)=x_p(t)+v'_x\,dt+\\
&\qquad +Z_1\cdot\sqrt{2D_Ldt}\cdot\frac{v_x}{v}-Z_2\cdot\sqrt{2D_Tdt}\cdot\frac{v_y}{v}\\
&y_p(t+dt)=y_p(t)+v'_y\,dt+\\
&\qquad +Z_1\cdot\sqrt{2D_Ldt}\cdot\frac{v_y}{v}+Z_2\cdot\sqrt{2D_Tdt}\cdot\frac{v_x}{v}
\end{aligned} \qquad (3)$$

where $x_p(0)=x_0$, $y_p(0)=y_0$ is particle's starting position;

$$v'_x = v_x + \frac{\partial D_{xx}}{\partial x} + \frac{\partial D_{xy}}{\partial y}\,; \qquad v'_y = v_y + \frac{\partial D_{yx}}{\partial x} + \frac{\partial D_{yy}}{\partial y}$$

and $v = \sqrt{v^2{}_x + v^2{}_y}$ are correction terms when dispersion is included; Z_1 and Z_2 are random numbers generated from Gaussian standard distribution.

2.2 Defining groundwater age

As previously mentioned, this paper applies direct simulation of groundwater age using Lagrangian approach and RWTP but no concentration calculation is needed as we only use the Eq. (3) for water particles position.

Numerical solution for groundwater flow calculation – program FI (our personal software), which uses finite elements method, has been modified to implement calculation of groundwater age.

First step is to have velocity field calculated and then additional subroutine is programmed to make water particles (all grid nodes) to do the back stepping using reversed velocity field. Simulation logic works in a way as if from each node there is particle traveling back to the point of entry into the aquifer, and each time step is summarized. Finally when particle crosses the boundary of domain, counting is finished and final sum presents retention time of certain particle in underground at starting point. In other words those final sums are groundwater age at starting point node, and when described calculation is done for all nodes we have groundwater age distribution in whole domain. Modified expressions for “reverse” RWPT are shown by Eq. (4), and scheme showing how particles are driven back via streamlines in the simulation is shown on Figure 1.

$$\begin{aligned} x_p(t+dt) &= x_p(t) - v'_x\,dt - \\ &\quad - Z_1 \cdot \sqrt{2D_L dt} \cdot \frac{v_x}{v} + Z_2 \cdot \sqrt{2D_T dt} \cdot \frac{v_y}{v} \\ y_p(t+dt) &= y_p(t) - v'_y\,dt - \\ &\quad - Z_1 \cdot \sqrt{2D_L dt} \cdot \frac{v_y}{v} - Z_2 \cdot \sqrt{2D_T dt} \cdot \frac{v_x}{v} \end{aligned} \qquad (4)$$

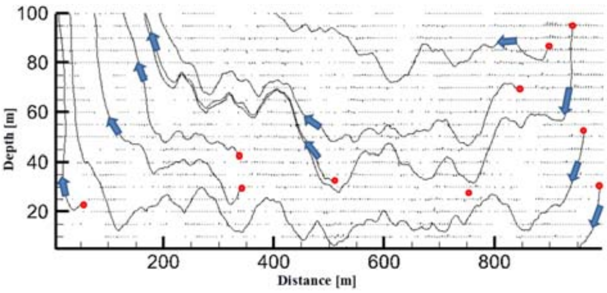

Fig. 1 Simulation scheme

2.3 Probability distribution of groundwater age

Modelling of flow and transport always carries certain uncertainties that need to be taken into account. As calculated velocity field is the most important input for the equation of sediment, then it is precisely necessary to analyse the impact of different velocity distributions that is due to the influence of heterogeneity.

We used a stochastic modelling, which then results in a solution in the form of mean values and the corresponding standard deviation. Monte Carlo method has been used for the case of low heterogeneity ($\sigma_y{}^2=0{,}1$) and medium heterogeneity ($\sigma_y{}^2=1{,}0$). Hundred simulations for hydraulic conductivity field have been performed using software Hydro_gen [15], and for each of them groundwater age calculation has been done and statistically processed to define fields of average groundwater age and associated standard deviations.

For chosen points (nodes) groundwater age probability density function may be calculated and more forward groundwater age probability is estimated in those points using some threshold expected ages as shown on Figure 2.

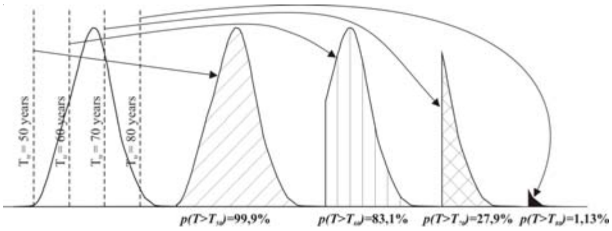

Fig. 2 Calculation of groundwater age probability from PDF at certain point

3. EXAMPLE SIMULATION

3.1 Synthetic example conditions

Numerical model for simulation of groundwater age developed in the previous section is applied to an example of aquifer scheme shown at Figure 3. The domain geometry and boundary conditions are identical for three different hypothetical aquifer systems: a uniform aquifer, an aquifer system with high permeability layer at lower level and heterogeneous one. These configurations are similar to what Goode used in his Direct simulation of groundwater age [2], along with Freeze and Witherspoon [16] before him in a landmark series of paper studying the regional groundwater flow.

The left, bottom and right boundary are impermeable. On top boundary left *9/10* of boundary have imposed flux and right *1/10* have imposed potential. Molecular diffusion, D_m $[m^2/s]$ and coefficients of longitudinal and traversal dispersion α_L and α_T [*m*] are chosen to be alternated for each type of aquifer, and some results are given afterward.

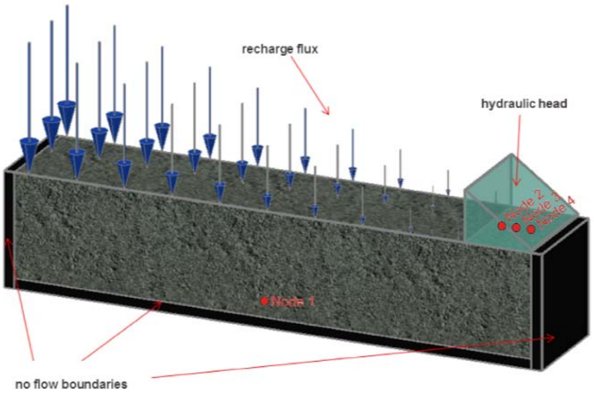

Fig. 3 Aquifer system scheme

3.2 Homogeneous aquifer and layered aquifer system

Examples presented in Figure 4 show how is groundwater age distributed for homogeneous aquifer and two layers aquifer with lower one having higher conductivity for transport driven both by advection and dispersion. Molecular diffusion is set to $D_m = 6*10^{-10}$ [m^2/s] and coefficients of longitudinal and traversal dispersion are $\alpha_L=10$ [*m*] and $\alpha_T=0{,}01$ [*m*], conductivity of homogenous one is $K=10^{-6}$ [*m/s*] same as upper part of layered one and lower part is $K=10^{-5}$ [*m/s*].

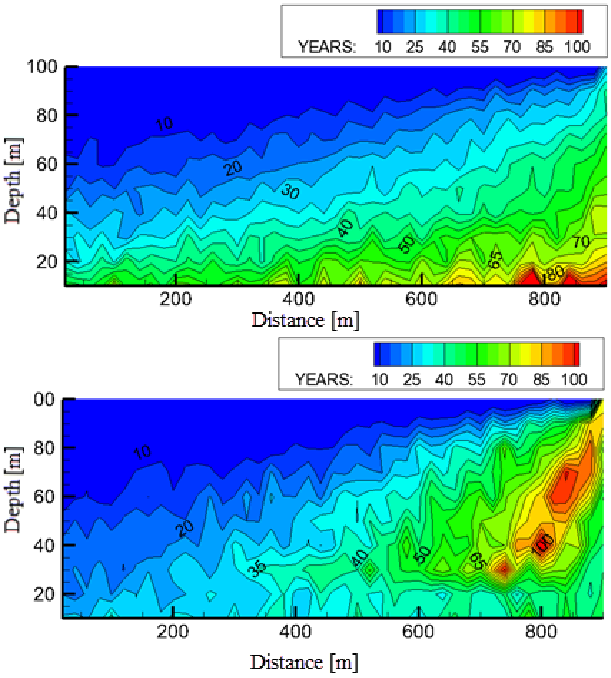

Fig. 4 Contour lines for groundwater age in a) homogenous aquifer; b) two layers aquifer

3.3 Heterogeneous aquifer systems

For heterogeneous aquifer system denser mesh was used in order to simulate different conductivity on each element and slightly different parameters of dispersion are chosen in order to maintain common Peclet's number in underground: $Pe_x=100$ and $Pe_y=1000$.

Parameters used for dispersion are $D_m=1{,}16*10^{-10}$ [m^2/s], $\alpha_L=0{,}005$ [*m*] and $\alpha_T=0{,}0005$ [*m*]. For generating random conductivity field we used average value $K=10^{-6}$ [*m/s*], correlation lengths are *20* [*m*] in *x* and *y* direction, and 2 different variances for low ($\sigma_y{}^2=0{,}1$) and medium heterogeneity ($\sigma_y{}^2=1{,}0$). After applying stochastic analysis results are given as mean groundwater age field and belonging standard deviation for low heterogeneity in Figure 5, and for medium heterogeneity in Figure 6.

As we used $K=10^{-6}$ [*m/s*] for average value when generating conductivity field, it can be noticed that mean groundwater age in heterogeneous aquifer fluctuates around the lines in solution for homogenous aquifer, and respectively those fluctuations are higher in medium heterogeneity case. Heterogeneous aquifer has jagged layers due to those fluctuations as a result of simultaneously influence of heterogeneity and dispersion.

Following the methodology described before, probability distribution for groundwater age is calculated in chosen 4 nodes (Figure 3). Three nodes are in the right upper corner where water age might be of biggest concern in case of using that water or estimating the level of pollution and one node is picked in the middle of aquifer to show the difference. In low heterogeneity case, most of PDFs were very similar to the Gaussian, and in medium heterogeneity case it was more like log-normal PDF caused by expanding the range of values due to higher variance. Cumulative distribution functions for groundwater age in both heterogeneity cases are shown in Figures 7 and 8.

There are few differences between nodes 1, 2 and 3 as they have similar streamline conditions, while node 4 which is physically closer to 2 and 3 than node 1, has rather higher values of groundwater age. Reason for this behaviour lies in streamlines which for node 4 do longer travel paths, going into the deeper layers, while particles coming out at nodes 2 and 3 mostly stay in upper layers and therefore have fewer years.

From calculated cumulative distribution functions one can clearly read out the probability of having water at possible intake of chosen age. For instance node 4 in most realizations has age higher than *100* years. In respect of the heterogeneity impact on the distribution itself it is obvious how values are more expanded, and with it the risk connected to groundwater age might be also higher.

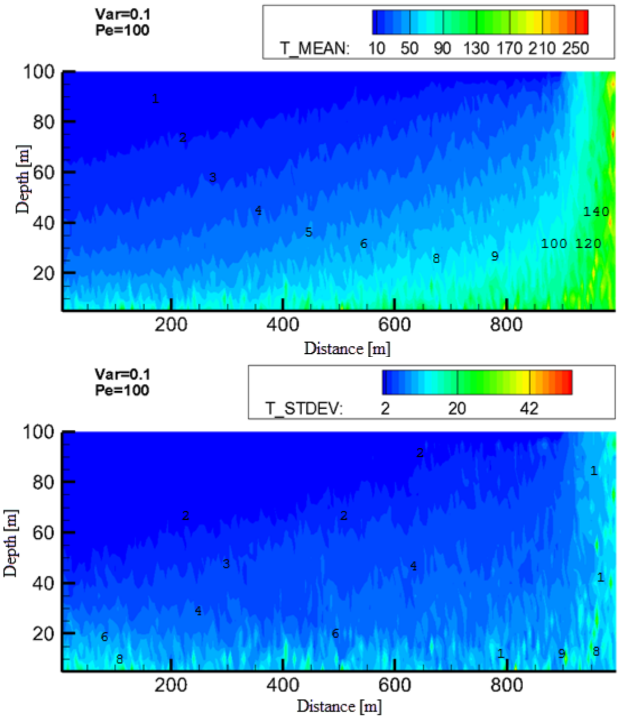

Fig. 5 Mean groundwater age field and standard deviation for σ_y^2=0,1

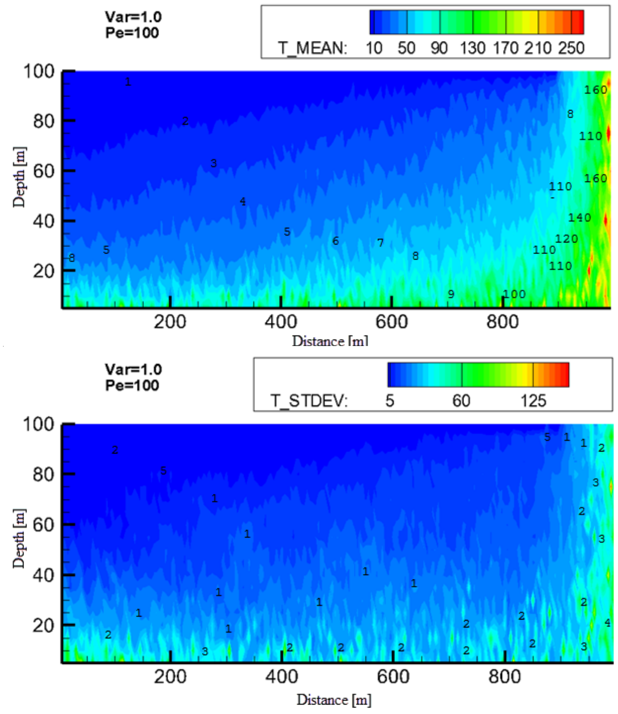

Fig. 6 Mean groundwater age field and standard deviation for σ_y^2=1,0

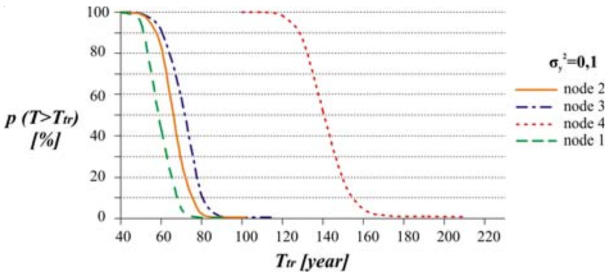

Fig. 7 Groundwater age probability at four different nodes for σ_y^2=0,1

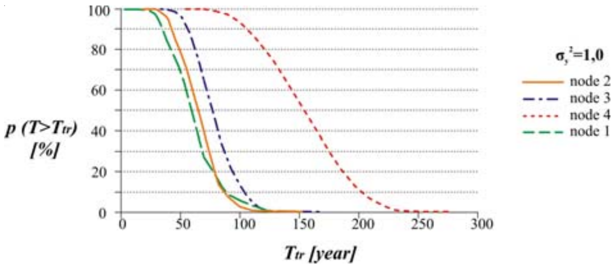

Fig. 8 Groundwater age probability at four different nodes for σ_y^2=0,1

4. CONCLUSION

Numerical model is developed using Lagrangian approach, where groundwater age is calculated as summed up traveling time of certain particles, when performing “reverse” random walk particle tracking method. This paper has shown that groundwater age directly depends on velocity field and therefore it is significantly influenced by heterogeneity of porous media. Hence, increased heterogeneity increases the residence time of water in the underground. Therefore, we can say that by taking the model for a homogeneous field in case of need for a simpler calculation, obtains lower values of age, which are on the safety side. This approach allows to obtain estimates of probability, and they give a range of values that can be expected and thus provide better decision support.

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UTJECAJ HETEROGENOSTI NA STAROST PODZEMNIH VODA

SAŽETAK

Starost podzemnih voda se promatra kao važno svojstvo vodnih resursa i može indicirati njihovu kvalitetu. U podzemlju veliki problem predstavlja nedovoljan broj mjerenja koji se mogu koristiti u direktnim simulacijama starosti podzemnih voda. Numerički model u ovom radu koristi Lagrange-ov pristup ("random walk particle tracking") u kojem je starost dobivena iz funkcije vremena putovanja raznih čestica za procese advekcije i disperzije. Za taj model proračun tečenja služi kao osnovni ulaz, a poboljšanje postojećeg modela tečenja je bila nužnost za dobivanje korektnih simulacija s kontinuiranim poljima brzina. Sintetički primjeri su napravljeni, za homogene, uslojene i heterogene akvifere. Za heterogeni akvifer napravljena je stohastička Monte-Carlo analiza u kojem je starost podzemnih voda prikazana pomoću prva dva momenta i funkcije gustoće vjerojatnosti. Primjena rezultata se može koristiti u procjeni očekivane starosti na danoj lokaciji na kojoj se koristi voda za piće. Zbog toga distribucija vjerojatnosti starosti podzemnih voda može poslužiti kao alat i metoda da se procijeni nivo autopurifikacije akvifera ili pak definira nivo tretmana vode prije njenog korištenja.

Ključne riječi: *starost podzemnih voda, Lagrange-ov pristup, random walk particle tracking, heterogenost, Monte Carlo simulacije, distribucije vjerojatnosti starosti podzemnih voda.*