

AN ASSESSMENT OF PARTICLE DISORDER EFFECTS ON SMOOTHED PARTICLE HYDRODYNAMICS SIMULATIONS OF TRANSPORT IN HETEROGENEOUS POROUS MEDIA

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ABSTRACT

Local-scale heterogeneity in natural aquifers plays a key role in solute mixing and chemical reactions. The incorporation of this scale of heterogeneity in traditional grid-based methods is difficult because of large computational costs and because of their poor accuracy in the advective-dominated transport found in most practical problems. Particle methods are an attractive alternative to simulate this kind of problem because of their natural ability to both simulate solute advection, and to adapt to irregular geometries and flow conditions, as well as their relatively low demand of computational power. However, it is difficult to incorporate and resolve solute mixing and dilution in traditional particle methods.

In this paper we explore the use of smoothed particle hydrodynamics (SPH) methods to simulate solute transport in heterogeneous geological formations. SPH methods are able to handle solute mixing and dilution in a natural way. In this article we review some of the important characteristics of the method and we evaluate its advantages and disadvantages for the simulation of solute transport that incorporates local-scale mixing.

1. INTRODUCTION

Our main objective is to develop a methodology to perform accurate numerical simulations of reactive transport in heterogeneous aquifers. In particular we are interested in capturing the effect of pore-scale dispersion and Darcy's scale velocity variability on solute mixing and dilution. There is substantial evidence that those are important processes that control reactive transport in natural aquifers, e.g. biodegradation reaction rates are controlled by mixing of chemical compounds. Mixing occurs when material lines are stretched by local velocity variability resulting in an increased area for diffusion. (Weeks and Sposito, 1998).

Traditionally numerical simulations of reactive transport in aquifers have been performed using grid or mesh based methods, e.g. finite difference, finite volume, or finite element. Those techniques present several problems for the accurate simulation of solute migration in highly heterogeneous velocity fields as found in real scenarios. First, the resolution of grid based methods is restricted by cell size, so the computational cost of accurate simulations in large domains is prohibitive for real scenarios, even considering the power of current computers. Second, the numerical solution of the advection-dispersion equation (ADE) under field conditions is very challenging for traditional grid based methods. Under those conditions solute transport is typically advection-dominated, and grid and mesh-based methods are often affected by numerical dispersion that can greatly enhance the rate of mixing and dilution. Therefore, it is difficult to estimate if the dilution of solute in the results of those simulations is due to physical mixing or artificial numerical dispersion (Cirpka et al., 1999).

Discrete particle tracking methods have been used in several studies to simulate solute transport in aquifers (e.g. Tompson and Gelhar, 1990; Tompson and Dougherty, 1992; Tompson, 1993). In those simulations each particle has a certain solute mass and negligible volume. Solute concentration is computed as the spatial average of solute mass in a given volume (grid). The solute migration is simulated by tracking the position of solute particles carried by Darcy's velocity. To incorporate local-scale dispersion and velocity variability at the subgrid-scale these methods use a random-walk approach where the displacement of a particle after a time step is given by a deterministic component and a random component that is a function of the local-dispersion or modelled subgrid-variability. The combined use of particle tracking and random-walk has been used to successfully simulate large-scale problems and to estimate first moments of the solute plume (location of center of mass and plume spreading). Mixing can be incorporated in those methods by mapping solute concentration onto a grid to redistribute the solute mass. That approach has several disadvantages such as: concentration averaging on a grid introduces numerical mixing that is very difficult to estimate, the construction of a grid that can be difficult in domains with irregular geometries, and reaction rates of chemical reactions cannot be computed in individual particles.

There are other types of particle methods based on a continuum spatial approximation, e.g. vortex methods (Rosenhead, 1930; Cottet and Koumoutsakos, 2000), particle strength exchange (PSE) (Degond and Mas-Gallic, 1989; Zimmermann et al., 2001), and smoothed particle hydrodynamics (SPH) (Gingold and Monaghan, 1977; Lucy, 1977). In these methods the value of an unknown at a spatial location is computed as the convolution of proximal particle locations and a shape function (Brackbill, 2005). These types of particle methods are very attractive to simulate continuum heterogeneous flow phenomena as solute transport in aquifers because they are naturally adaptive, efficient, stable, and accurate (Koumoutsakos, 2005). On the other hand, these methods have difficulty accommodating particle distortion caused by non-uniform velocity fields. The error introduced by particle distortion is difficult to evaluate and depends upon the dynamics of the simulated system (Monaghan, 2005).

The objective of this article is to study the use of a particle method based on SPH to simulate migration and dilution of solute plumes in heterogeneous aquifers. In section 2 we present a summary of the mathematical formulation of SPH methods and their implementation. We analyse the results of some numerical experiments in section 3. Finally, in section 4 we establish some conclusions particularly focused upon the application to reactive transport simulation and propose possible future research.

2. SMOOTHED PARTICLE HYDRODYNAMICS

Smoothed particle hydrodynamics methods were independently developed by Gingold and Monaghan (1977) and Lucy (1977) as a simple method to faithfully reproduce the equations of fluid dynamics of some astrophysical problems. SPH methods have since been used to simulate problems in diverse domains such as: star formation and collisions, geophysical problems, elasticity and fracture of materials, pore-scale dispersion, etc (Monaghan, 2005). Below we give a brief summary of the mathematical description of the method and some of its main features. Complete reviews of the subject are presented in Monaghan (1992) and Monaghan (2005).

2.1 Mathematical background

In the SPH formulation the integral interpolant at position \mathbf{r} of any variable A is expressed as (Monaghan, 1992)

$$A(\mathbf{r}) = \int A(\mathbf{r}') W(|\mathbf{r} - \mathbf{r}'|, h) d\mathbf{r}' \quad (1)$$

where W is a spheric interpolation kernel, and h is a distance scale related to the domain of influence of the kernel and that is commonly denoted as the kernel smoothing length. The kernel function W must satisfy the following conditions

$$\int W(|\mathbf{r} - \mathbf{r}'|) d\mathbf{r}' = 1 \quad (2)$$

$$\lim_{h \rightarrow 0} W(|\mathbf{r} - \mathbf{r}'|, h) = \delta(\mathbf{r} - \mathbf{r}') \quad (3)$$

where δ is the Dirac delta function. Note that the SPH formulations allows h to vary in space and time. This last property can be used to increase the resolution and adaptivity of the method in problems with irregular particle distribution (Monaghan, 1992). For numerical implementation the integral in (1) is approximated by a discrete summation over a set of particles, i.e.

$$A(\mathbf{r}) = \sum_b \frac{m_b}{\rho_b} A_b W(|\mathbf{r} - \mathbf{r}_b|, h) \quad (4)$$

where m_b and ρ_b are the mass and density of the fluid volume associated to particle b , A_b is the value of any variable A at \mathbf{r}_b , and $W(|\mathbf{r} - \mathbf{r}_b|)$ is a function with finite compact support, i.e. $W \neq 0$ only in a closed, finite region of the spatial domain. Therefore, the summation in (4) occurs over all particles within the support volume of the kernel centered at position \mathbf{r} .

In some cases it is more convenient to define a new variable $n_b = \rho_b / m_b$ to replace the volume of fluid associated to particle b , $V_b = m_b / \rho_b$, in (4) to obtain (Tartakovsky and Meakin, 2005)

$$A(\mathbf{r}) = \sum_b \frac{A_b}{n_b} W(|\mathbf{r} - \mathbf{r}_b|, h) \quad (5)$$

One of the most important properties of SPH methods is that derivatives of spatial variables can be easily computed. For example, if W is differentiable, the gradient of A is expressed as

$$\nabla A(\mathbf{r}) = \sum_b \frac{A_b}{n_b} \nabla W(|\mathbf{r} - \mathbf{r}_b|, h) \quad (6)$$

Similarly (Chaniotis et al., 2002),

$$\frac{\partial^2 A(\mathbf{r})}{\partial x_i \partial x_j} = \sum_b \frac{A_b}{n_b} \frac{\partial^2 W(|\mathbf{r} - \mathbf{r}_b|, h)}{\partial x_i \partial x_j} \quad (7)$$

2.2 Solute transport using SPH

To simulate solute transport in aquifers using SPH we solve two equations. First, fluid particles are moved due to the action of Darcy's scale velocity, \mathbf{v}_D , such that

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_D(\mathbf{x}_p) \quad (8)$$

where \mathbf{x}_p is the position vector of particle p . Equation (8) can be accurately integrated on a staggered grid using the semi-analytical approach developed by Pollock (1988) to estimate fluid particle positions as function of time.

The exchange of solute mass between particles due to local-scale dispersion can be incorporated by solving

$$\frac{dC_i}{dt} = \nabla \cdot (D \nabla_i C) \quad (9)$$

where C_i is the solute concentration at particle i , and we have assumed that local-dispersion is isotropic, so can be modeled by an scalar coefficient, D . Equation (9) can be solved by directly replacing (6) and (7) (Chaniotis et al., 2002). However, the resulting expression is very sensitive to particle disorder. A better way to solve (9) is to use an integral approximation of the dispersive fluxes on the right side of (9), as explained by Clearly and Monaghan (1999); and Jubelgas et al., (2004). Using this last approach, (9) is solved by integrating (Tartakovsky and Meakin, 2005)

$$\frac{dC_i}{dt} = \sum_j \frac{(D_i n_i + D_j n_j)(C_i - C_j)}{n_i n_j |\mathbf{r}_i - \mathbf{r}_j|^2} (\mathbf{r}_i - \mathbf{r}_j) \cdot \nabla_i W(|\mathbf{r}_i - \mathbf{r}_j|, h) \quad (10)$$

in time. Zhu and Fox (2001) and Tartakovsky and Meakin (2005) have used this expression to simulate solute dispersion at the pore-scale. Recently, Español and Revenga (2003) and Monaghan (2005) have derived integral expressions to compute second derivatives in the more general case of anisotropic dispersive fluxes.

2.3 Effect of particle disorder on the accuracy of the SPH solution

Particle methods based on interpolant approximations are affected by two main sources of error. First, the continuum approximation in (1) introduces a smoothing error. Second, the transformation of (1) into the discrete expression (4) introduces a discretization error (Brackbill, 2005; Quinlan et al., 2005). Quinlan et al. (2005) have shown that for uniformly particle spacing the error estimate, e , for SPH methods is given by

$$e < C_1 \left(\frac{\eta}{h} \right)^y + C_2 h^2 \quad (11)$$

where η is the distance between particles, C_1 and C_2 are coefficients that depend only on the smoothness of the data, $y > 0$ is a constant related to the smoothness of the kernel. The first term in (11) is related to the discretization error and the second one to the smoothing error.

There are situations where the error is controlled by the ratio η/h (i.e. the number of particles in the kernel support volume) and others where the second term depending only in h is dominant. In general, for regularly distributed particles the error is controlled by the discretization error, so the method converges as $h \rightarrow 0$. Clearly and Monaghan (1999) show that for a set of equispaced or random uniformly distributed particles the error of the SPH formulation (10) converges with h^2 . The situation is much more complicated when particles are non-uniformly distributed. Quinlan et al. (2005) have shown that in that case it is difficult to identify the leading term in (11). They have shown that in some situations the error decreases as h increases for a given ratio η/h .

This analysis indicates that irregular distribution of particles due to action of the heterogeneous velocity field in our simulations can degrade the accuracy of the SPH method used to solve (9). It also indicates that for a given number of particles with irregular locations it is possible to obtain higher accuracy by modifying h or η/h .

3. NUMERICAL EXPERIMENT

We set up a test scenario to study the performance and accuracy of the SPH method to account for local-dispersion under typical field conditions. In particular, we are interested in estimating the error introduced by particle disorder due to advective transport and to verify error analysis discussed above. To do that we first generate a velocity field by solving the flow equation using a synthetically generated random hydraulic conductivity field. Then, we simulate solute transport in two scenarios: one considering only advection and a second one considering only local-dispersion.

3.1 Velocity field generation

We generate a stationary two-dimensional random hydraulic conductivity field using the method described by Robin et al. (1993). The statistics of the generated random field correspond to the statistics of field data analysed by Wierenga et al. (1991). The statistics of $Y=\ln(K)$ are: mean value $\langle Y \rangle = 6.02$ (where K is in cm/day), variance $\sigma_Y^2 = 1.46$, and isotropic correlation lengths $\lambda_x = \lambda_y = \lambda = 2.82$ (m). We used a Gaussian covariance model with integral scale $I = \lambda \sqrt{\pi}/2 = 2.5$ (m). In what follows we normalize length and time scales using the integral scale I . We generated a $400I \times 140I$ random field with 2000×700 square cells of size $I/5$. Previous studies have shown that this grid resolution is sufficiently fine for transport simulations (Chin, 1997).

We solved for steady-state confined saturated flow in the generated hydraulic conductivity field. As boundary conditions we used constant head on the left and right, and no-flux on top and bottom sides of the domain. To avoid spurious correlations from the random field generator, we compute the hydraulic head in an embedded 1602×602 cell subdomain of the original grid. We used the head solution and Darcy's law with harmonic averaging of block hydraulic conductivities to compute a staggered velocity field with components at the edges of each cell. The resulting velocity field has mean value $\mathbf{U} = (0.02, 0.0)$ [L/T], variance $\sigma_{v_x} = 2E-4$ and $\sigma_{v_y} = 9E-5$, and maximum value in the x-direction, $v_x^{max} = 0.18$ [L/T]. The computed velocity has a small maximum divergence, $(\nabla \cdot \mathbf{v})_{max} = 4.35E-10$. Figure 1 shows the spatial variation of the magnitude of the generated velocity field.

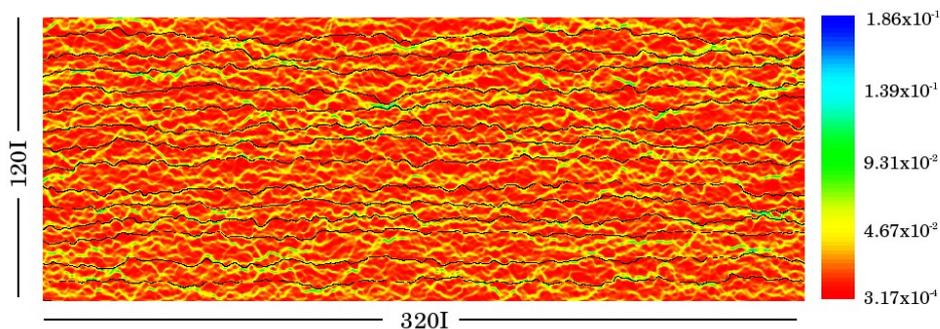


FIGURE 1: Velocity magnitude (color scale) and streamlines (black lines) of generated velocity field. Velocity field is $320 \times 120 \ln(K)$ integral scales, I .

3.2 Advective transport

We first simulate a purely advective transport problem. We initially distribute particles in a rectangular region with origin $(x_0, y_0) = (44I, 40I)$ and limit $(x_{limit}, y_{limit}) = (144I, 100I)$. We distribute 37500 particles on an equispaced rectangular lattice with spacing I , i.e. there are 250 particles in x direction by 150 particles in y direction. We simulate the advective transport of this particle cloud for a dimensionless time $\tau = U_x t / I = 250$. Figure 2 shows the final distribution of particles. We observe that particles are very irregularly distributed due to the differences in velocity and that the longitudinal dimension of the cloud is twice the initial size of the original rectangular cloud.

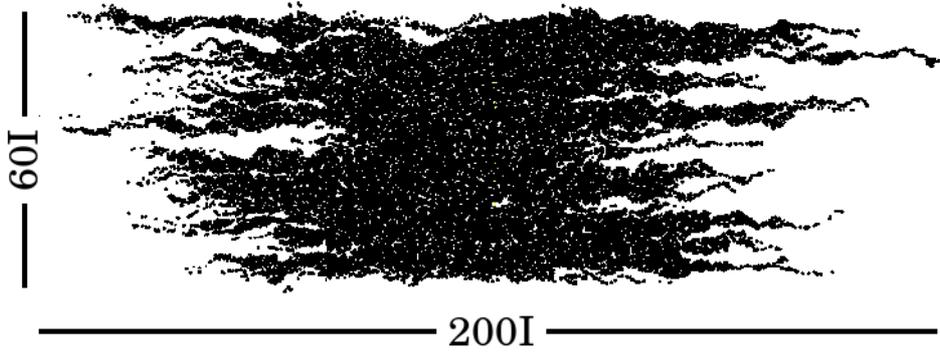


FIGURE 2: Spatial particle distribution of initial rectangular particle cloud after traveling $250 \ln(K)$ integral scales, I .

3.3 Effect of particle disorder in accuracy of SPH solution

It is difficult to estimate the error of the numerical solution of solute transport in heterogeneous velocity fields because of the lack of analytical solutions. Therefore, to estimate the error that affects the SPH formulation (10) we performed a simple numerical experiment: we used the advected particle distribution shown in Figure 2 to simulate a situation where we only considered local-dispersion. As an initial condition we used a Gaussian plume at the center of the particle cloud at position $\mathbf{r}_0 = (196I, 70I)$, such that the initial concentration at position \mathbf{r} is given by $c(\mathbf{r}, t=0) = c_0 \exp(-|\mathbf{r} - \mathbf{r}_0|^2 / (2\sigma_0^2))$. This simple initial condition allowed us to compare the numerical results with an analytical solution for isotropic dispersion D , given by $c(\mathbf{r}, t) = [(c_0 \sigma_0^2) / \sigma^2] \exp(-|\mathbf{r} - \mathbf{r}_0|^2 / (2\sigma^2))$, where $\sigma^2 = \sigma_0^2 + 2Dt$. We choose the value of D such that the Péclet number, $Pe = UI / D \approx 20$. Note that this is a relatively low value of Pe for most field problems, so it gives us a conservative estimate of the error when solving local-dispersion. In our simulations we have used spline kernels of third order W3, and fourth order W4, that have compact support $2h$ and $2.5h$, respectively (Price, 2004). To minimize errors associated with the time integration of (10) we used a fourth-order explicit Runge-Kutta integrator with a very small time step, Δt , such that $U \Delta t / I = 0.04$.

Figure 3a shows the L_∞ norm of the relative error between the numerical and the analytical solutions, $\epsilon = (c_n - c_a) / c_0$. We observed that the numerical error for all combinations of kernels and ratio $\beta = h / \eta$ are relatively large. At the same time we observe that it is possible to reduce the error by increasing the number of particles in the kernel's

support volume (i.e. ratio β) while keeping the same total number of particles. It is important to notice that the increment in β means that more particles contribute to the sum in (10), so the computational cost increases. On the other hand, the memory requirement, which depends upon the total number of particles, is constant. This figure also shows that for this particle distribution the choice of β has a larger effect on the accuracy of the solution than choice of the kernel function.

To isolate the contribution of particle disorder to the error we simulate a second local-dispersion scenario with the same parameters as the first simulation except instead of using the disordered particle distribution that followed the advection step (Figure 2) we now use a uniform particle distribution. Figure 3b shows a comparison of the relative error for both scenarios. We observe that the errors for simulations using irregular particle locations is between two or three orders of magnitude higher than the simulations using regular particle spacing.

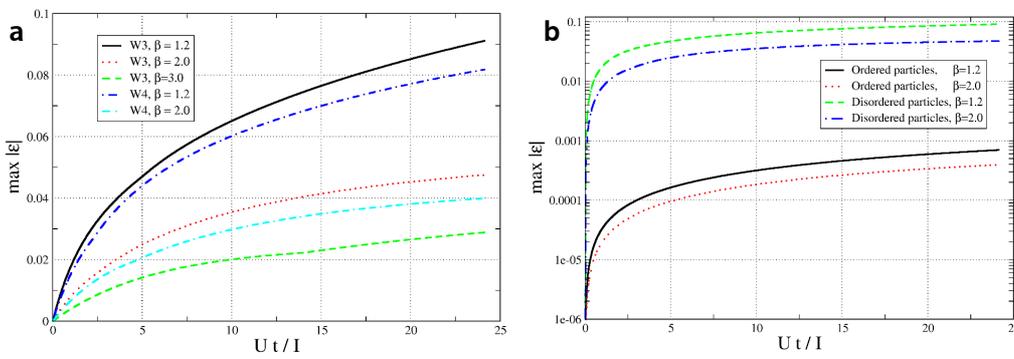


FIGURE 3: Comparison of error between numerical and analytical solution. a) For different combinations of kernel and ratio of smoothing length and initial particle spacing, $\beta = h/\eta$. b) For disordered and ordered particle locations using W3 kernel.

4. CONCLUSIONS

Although smoothed particle hydrodynamics are a promising method to simulate solute transport in groundwater, as with many particle methods, they suffer from errors when particles are nonuniformly distributed. We show that the accuracy of the method can be improved by varying the number of particles that fall within the support volume of the smoothed particle kernel. As clustering and channeling of particles is common in simulations of heterogeneous porous media, methods that can identify and correct for particle disorder such as adaptive kernel resolution and particle re-initialization should be explored in future research.

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