# ANTI-DIFFUSION MODELING USING A NON-LOCAL CENSORED RANDOM WALK SCHEME

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## ABSTRACT

This paper extends the Reversed Time Particle Tracking Method of Bagtzoglou (2003) and presents a novel methodology for time reversal in groundwater transport simulations. The basis of the proposed scheme for anti-diffusion is a continuous time, censored, non-local random walk capable of tracking groundwater solute concentration profiles over time. Our analysis leads to the conclusion that an adaptive (decreasing) time-stepping scheme is necessary in order to maintain a constant amount of anti-diffusion. More specifically, we study the interrelations between the following parameters: time-step evolution versus time or number of steps; variance evolution (decrease rate); and total time or total number of steps required to reach a fully anti-diffused solution. The approach is shown to be quite efficient (every 80 time steps an eight-fold reduction of the variance is attained) and is also asymptotically exact. Our method is applied to one-dimensional and two-dimensional isotropic transport of conservative solutes in spatially invariant and variant groundwater flow fields with great success.

## 1. INTRODUCTION

In view of increasing demands for clean drinking water, it is highly desirable to identify pollution sources accurately, as well as to backtrack the pollution source, to recover the spatial extent the plume at different times, and ultimately, to reconstruct the contamination plume release time history. This can be formulated as an advection-diffusion *inverse problem*. Its difficulty is compounded by the fact that geologic media are highly heterogeneous. In this context, the objectives of this paper are to contribute, first, to the problem of *source position identification*.

It is common practice for hydrogeologists to use computer simulation models in order to assess and study potential sources of contamination. Each and every one of the probable locations is considered as an *a priori* known feasible solution. Extensive simulations running forward in time provide a good understanding of how close to the present contaminant spatial configuration this potential source leads. This process, repeated as many times as the number of potential sources, ultimately pinpoints the most probable solute source. The disadvantage, associated with this methodology, is the extensive computational burden imposed. Backward or reversed time simulations employing **conventional** modeling approaches have been unsuccessful for solute source identification for the following reasons: 1) Finite difference and finite element methods constitute numerical mass transport models of unstable behavior, when used for backtracking of present contaminant configurations. The stability criteria are, for all practical purposes, restrictive enough to make their use non-feasible. Atmadja and Bagtzoglou (2001a) have demonstrated this unstable behavior for a finite difference transport model. 2) Particle tracking methods (PTMs), though effective in handling time reversal for purely advective contaminant transport, are incapable of treating dispersive and/or reactive transport.

Even though direct approaches that perform time inversion in the context of contaminant source identification have enjoyed visibility lately, their wide spread use is still limited due to the sophistication and non-conventional nature of the methods involved. Thorough reviews of the field can be found in the papers by Morrison (2000a; b; c), Atmadja and Bagtzoglou (2001a; b), and Bagtzoglou and Atmadja (2003; 2005). The purpose of this paper is to build on the Reversed Time Particle Tracking Method (RTPTM) of Bagtzoglou (2003) and present a novel methodology for time reversal in groundwater transport simulations. The basis of the proposed scheme for anti-diffusion is a continuous time, censored, non-local random walk capable of tracking groundwater solute concentration profiles over time. Moreover, and contrary to the RTPTM of Bagtzoglou (2003) it does not require an adaptively increasing particle resolution, which may render the computational power requirements formidable.

## 2. THE REVERSED TIME PARTICLE TRACKING METHOD

The RTPTM modifies the Random Walk Particle Tracking Method (RWPTM) step equation by introducing a variance or second moment minimization approach. Diffusion can be expressed in terms of the spatial variance of the particle cloud as

$$2D = \frac{d}{dt}(\sigma^2). \tag{1}$$

The spatial variance or normalized second order moment matrix, corrected for the center of mass, reads

$$\sigma^2 = \frac{1}{M}\int_{\Omega} C(x-\bar{x})(x-\bar{x})^T d\Omega = \sum_{i=1}^{N_p} \tilde{m}_i (x_i - \bar{x})(x_i - \bar{x})^T, \tag{2}$$

where $N_p$ is the number of particles in the system; $M = \sum_{i=1}^{N_p} m_i$ is the total solute mass within domain Ω; $\bar{x}$, $x_i$ are the position vectors for the plume center of mass and each individual particle, respectively; and $\tilde{m}_i = \frac{m_i}{M}$ is the normalized particle mass.

When the solute transport process advances forward in time, $D$ is a definite positive matrix, implying that the general 3D spread of solute about the center of mass $\bar{x}$ is increasing. Similarly, negative diffusion and time reversal can be easily implemented by decreasing the spatial spread of the particle cloud around its center of mass. The step equation for the RTPTM consists of the following set of equations:

$$\begin{aligned} X^n &= \bar{X}^n + F(\bar{X}^n, t_n) Q(t_n), \\ \bar{X}^n &= \bar{X}^{n+1} - A(\bar{X}^{n+1}, t_{n+1})\Delta t, \\ F(\bar{X}^n, t_n) \cdot F^T(\bar{X}^n, t_n) &= \sigma_n^2, \\ \sigma_n^2 &= \sigma_{n+1}^2 - 2\Delta t D, \end{aligned} \tag{3}$$

where vector $Q(t_n)= Q^n=R^nS^n$, $R^n$ is a normalized random vector with mean of zero and unit variance, and $S^n$ is a random sign (±) vector, both defined at time $t_n$.

Equation set (3) constitutes the backbone of the RTPTM, being easily reduced to their two- or one-dimensional (2D, 1D) forms. The method can be also applied to forward time simulations, by rearranging these equations, yielding results equivalent to the classical RWPTM. Consider a particle $p$, which at time $t_n$ has a position vector given by $X^n$. Assume further that this particle is displaced, according to the RTPTM and RWPTM step equations , to $X_*^{n+1}$ and $X_{**}^{n+1}$, respectively. If the two methods were to be equivalent the two positions should be equal, thus yielding

$$X^n + A(X^n,t_n)\Delta t + B(X^n,t_n)W(t_n) = \bar{X}^n + A(\bar{X}^{n+1},t_{n+1})\Delta t + F(\bar{X}^{n+1},t_{n+1})Q(t_{n+1}). \tag{4}$$

After some algebraic manipulations and assuming that the time step $\Delta t$ is sufficiently small, the following equivalence is obtained

$$\begin{aligned} B(X^n,t_n) &= \Phi(\varepsilon^n,t_n) + \Psi(\bar{X}^{n+1},t_{n+1}) \\ \Phi(\varepsilon^n,t_n) &= \frac{\varepsilon^n}{Z^n\sqrt{\Delta t}} + \frac{A^*(\varepsilon^n,t_n)\sqrt{\Delta t}}{Z^n} \\ \Psi(\bar{X}^{n+1},t_{n+1}) &= F(\bar{X}^{n+1},t_{n+1})\frac{R^{n+1}S^{n+1}}{Z^n\sqrt{\Delta t}} \end{aligned} \tag{5}$$

where an *eccentricity* vector

$$\varepsilon^n = \bar{X}^n - X^n \tag{6}$$

and a *differential flow* or *drift velocity* vector

$$A^*(\varepsilon^n,t_n) = A(\bar{X}^n,t_n) - A(X^n,t_n) \tag{7}$$

are introduced. Φ and Ψ are **non-local** matrices, depending on the eccentricity of a specific particle and the center of mass of the particle cloud, respectively. Equation set (5) proves the existence of matrices $B$, Φ and Ψ, which would ensure the equivalence of results in the classical RWPTM and the "forward-time" RTPTM approach.

## 3. THE REVERSE ANTI-DIFFUSION WALK APPROACH

We have recently developed a novel scheme using a "reverse", anti-diffusive particle random walk, in a Lagrangian framework. This scheme should achieve *source identification* without having to deal with ill-posed or poorly conditioned inverse PDE problems. Moreover, and contrary to the RTPTM of Bagtzoglou (2003) it does not require an adaptively increasing particle resolution, which may render the computational power requirements formidable. It is based on a "censored" random walk whose properties are tailored to produce just the right amount of "Fickian anti-diffusion", in order to force the present ("final") diffusion plume to refocus backwards in time, at the correct rate, towards its "initial state" or source. We name it "Reverse Anti-diffusive Walk" (RAW). The objectives are to generalize its use for heterogeneous field pollution with advective transport and tensorial dispersion. The particle-based RAW scheme is now briefly described in the case of pure isotropic (anti)diffusion. Glimpses of the analytical theory are given in 1D; numerical results are displayed both in 1D and 2D.

## 3.1 Formulation of the particle-based anti-diffusive scheme

### *3.1.1 Continuous time formulation*

The basis of the anti-diffusion scheme is a continuous time, censored, non-local random walk (here described in the 1D case for simplicity):

$$dX(t)=\begin{cases}\sqrt{2D}\; dU(t)=\sqrt{2D}\;\xi(t)dt & if \quad S_{LOCAL}=-S_{GLOBAL} \\ 0 & otherwise\end{cases} \quad (8.1)$$

$$S_{LOCAL}=Sign(dU(t)) \quad (8.2)$$

$$S_{GLOBAL}=Sign\left(X(t)-\overline{X}(t)\right) \quad (8.3)$$

Several remarks are in order in regards to equations (8).

First, anti-diffusion is forced by the *minus* sign in "$S_{LOCAL}$= - $S_{GLOBAL}$". Secondly, non-locality is due to the fact that local displacement depends on mean displacement, or center of mass of the plume, via equation (8.3). Thirdly, although this scheme is formulated here in continuous time, it is physically more meaningful in discrete time (as will be seen later).

### *3.1.2 Discrete time formulation and adaptive time-stepping*

Using an explicit time discretization of equations (8) along with a specific adaptive time-step, $\Delta t = \Delta t_n$, we are able to show by probabilistic arguments that a constant anti-diffusion rate equal to $-D_I$ can be achieved, where $D_I$ may be different from the pseudo-diffusion rate $D_0$ that adjusts the intensity of jumps in the censored random walk. We obtain the following theoretical results based on random process theory. Briefly, constant rate anti-diffusion is achieved, with decreasing dispersion variance, as follows: $\sigma_X^2(t_{n+1})=\sigma_X^2(0)-2D_1\, t_{n+1}$, where ($t_n$) is a discrete time related to an adaptive time-stepping scheme ($\Delta t_n$). In the limit $n\to\infty$, we find $\Delta t_n \to 0$ and we obtain the asymptotic time: $t_n \to t_{SUP}=\sigma_X^2(0)/2D_1$. We can also deduce, from the maximum anti-diffusion time $t_{SUP}$, the maximum amount of variance reduction that has occurred during that time. The result is of the form: $\sigma^2(t_n)=\sigma_0^2-2D_1\,\Delta t_1\left(1-\beta^n\right)/(1-\beta)$, and satisfies $\lim_{n\to\infty}\sigma^2(t_n)=\sigma_{MIN}^2=0$.

This anti-diffusion procedure becomes 100% efficient in the limit as $n\to\infty$ and $\Delta t_n \to 0$, provided that $0 < \beta < 1$, which is always satisfied if $D_0 \le D_I$. Choosing $D_0 = D_I$ gives $\beta \approx 0.5947$; the variance reduction ratio is about 0.5% after 10 time steps, and on the order of $10^{-6}$ after only 25 steps.

# 4. NUMERICAL RESULTS: PLUME NARROWING & SOURCE FOCUSING

Figures 1 and 2 below illustrate the numerical implementation (in MATLAB™) of our anti-diffusion particle scheme in 1D and 2D. The program was also used to generate the "final" Gaussian plume. In all results below, *t* is "backward time", i.e., the plume evolves into the past as *t* increases.

## 4.1 1D results

In the 1D test presented here: $D_0 = 1$; $D_I = 0.1$; thus $\omega = D_I/D_0 << 1$. The adaptive time step was calculated numerically, i.e., based on the theoretical equations but using numerical moments of the particle cloud (not theoretical moments). The total number of adaptive anti-diffusion time-steps was $n_{MAX}$=50. The initial (or rather final) plume at time *t*=0 was Gaussian, with N=10,000 particles.

The 1D results indicate that: (i) for $\omega = D_1/D_0 \geq 1$ (not shown), concentration profiles are not Gaussian although they do converge to a Dirac function; (ii) for $\omega = D_1/D_0 << 1$, concentration profiles are near Gaussian at all times and they converge to a Dirac function at the source.

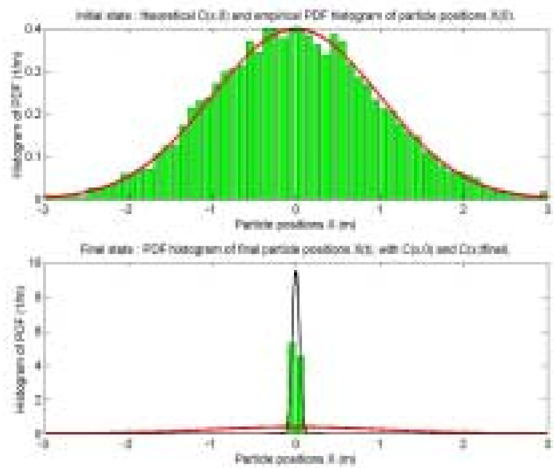

FIGURE 1. Particle distributions in 1D space. Top: "final plume" starting at $t = 0$. Bottom: "quasi-initial plume" after 50 adaptive anti-diffusion steps.

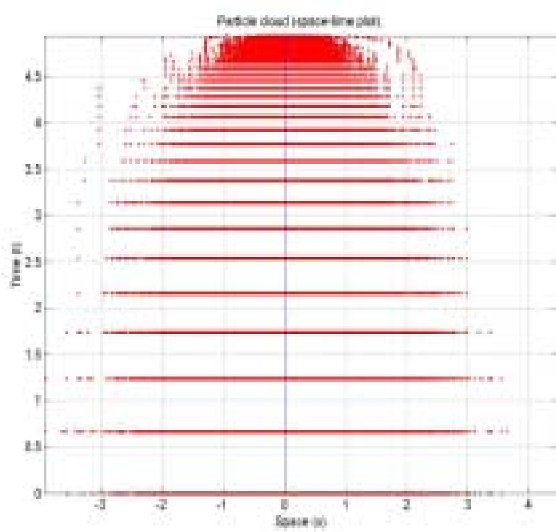

FIGURE 2. Space-time plot of 1D particle cloud during anti-diffusion. Bottom line: $t$=0 (final plume). Top line: narrow quasi-initial plume (after 50 steps).

### 4.2 2D isotropic results

Starting with a 2D isotropic Gaussian plume *C(x,y)*, we analyze in Figure 3 the plume as a particle histogram *vs.* radial distance to the center of mass (r). Indeed, if *C(x,y)* is bivariate Gaussian, *C(r)* must follow a Rayleigh distribution. It turns out that the Rayleigh distribution fits quite well the numerical plumes, i.e., they remain close to isotropic Gaussian as they become narrower during anti-diffusion (a rather satisfactory result). Finally, the analytical (theoretical) and computed (numerical) dispersion variance during the 2D isotropic anti-diffusion process dispersion variance decreases almost linearly with time, in an anti-Fickian fashion, as required. Figure 4 depicts the space-time particle plot for this 2D isotropic anti-diffusion problem.

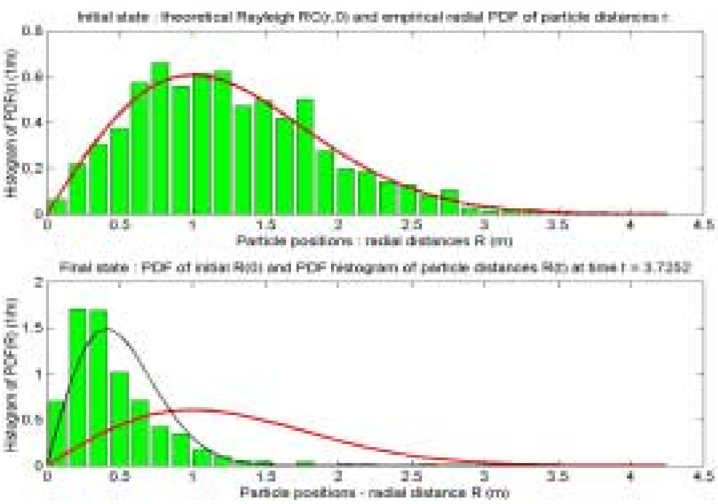


FIGURE 3. Radial particle plot, and fitted Rayleigh distribution, *C(r)*, during 2D anti-diffusion starting from Gaussian plume on top.

## 5. CONCLUSIONS

A novel methodology for time reversing in particle tracking methods was presented. A variance minimization procedure leading to a stochastic method, analogous to the RWPTM, capable of tracking back in time existing groundwater solute concentration profiles was developed. It is important to realize that, counter-intuitively, there exists a need to use more particles near the solute source in order to minimize the uncertainty involved. This would necessitate the implementation of adaptive approaches, whereby the number of particles involved in the simulation is increased as the plume is further tracked backwards in time.

This recognition led us to extend the RTPTM by introducing the RAW scheme for anti-diffusion, which is a continuous time, censored, nonlocal random walk capable of tracking groundwater solute concentration profiles over time. Our analysis leads to the conclusion that whereas the RTPTM requires adaptively an increasing particle resolution, an adaptive (decreasing) time-stepping scheme is necessary in order to maintain a constant amount of anti-diffusion for the RAW scheme.

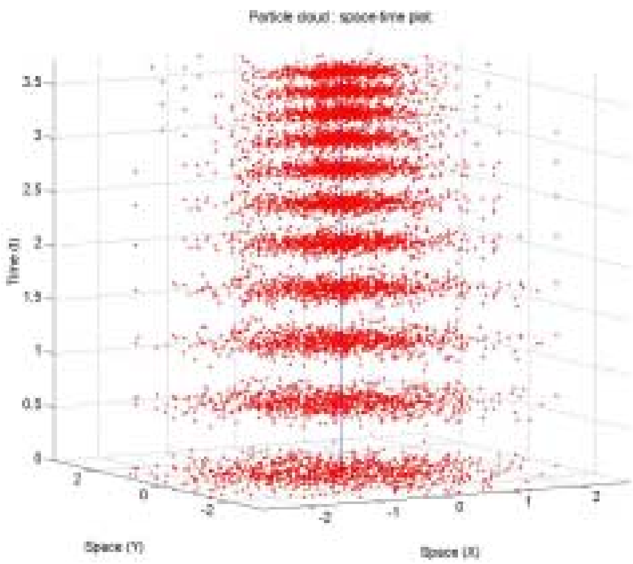


FIGURE 4. Space-time particle plot for 2D isotropic anti-diffusion problem (time is vertical).

To summarize, the proposed particle-based "RAW" scheme, with adaptive time-stepping, appears to be efficient in refocusing a present-day ("final") particle cloud back on the original point source at a near constant (fickian) anti-diffusion rate. Moreover, if the "observed" cloud is Gaussian, the intermediate particle clouds during the refocusing process are also nearly Gaussian.

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