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# A NON-FICKIAN, PARTICLE-TRACKING DIFFUSION MODEL BASED ON FRACTIONAL BROWNIAN MOTION

PAUL S. ADDISON,[1*] BO QU,[1] ALISTAIR NISBET[2] AND GARETH PENDER[2]

[1] *Department of Civil and Transportation Engineering, Napier University, Merchiston Campus, 10 Colinton Road, Edinburgh EH10 5DT, U.K.* [2] *Department of Civil Engineering, Glasgow University, The Rankine Building, Oakfield Avenue, Glasgow G12 8LT, U.K.*

## SUMMARY

The work is motivated by the recent discovery that ocean surface drifter trajectories contain fractal properties. This suggests that the dispersion of pollutants in coastal waters may also be described using fractal statistics. The paper describes the development of a fractional Brownian motion model for simulating pollutant dispersion using particle tracking. Numerical test cases are used to compare this new model with the results obtained from a traditional Gaussian particle-tracking model. The results seems to be significantly different, which may have implications for pollution modelling in the coastal zone. © 1997 John Wiley & Sons, Ltd.

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## 1. INTRODUCTION

In recent years, society's increasing environmental awareness coupled with global legislation has resulted in the pollution of river, estuarine and coastal waters becoming an important issue for water engineers. The need to predict the transport of pollutants has resulted in a rapid rise in the use of numerical models. Of the methods available, particle-tracking models are increasing in popularity owing to their ease of application and the well-known difficulties associated with numerical solutions (finite difference or finite element) to advection–diffusion equations,[1] particularly in areas where high concentration gradients exist, such as close to point sources.

Where the use of particle tracking models can provide valuable information to aid in problem analysis and engineering design, the understanding of the physical processes on which the models are founded remains limited. The potential for improvement is therefore considerable.

To date, the particle tracking models presented in the literature employ random Brownian motion to simulate turbulent diffusion.[2–7] Such models assume that particle tracks are neutrally persistent, i.e. a particle executes a simple random walk, showing no preference in its direction from step to step in the diffusion calculations. Field observations,[8–10] however, strongly indicate that particle movement is persistent, where the Lagrangian memory of the particle[11] plays an important role in

* Correspondence to: P. S. Addison, Department of Civil and Transportation Engineering, Napier University, Merchiston Campus, 10 Colinton Road, Edinburgh EH10 5DT, U.K.

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dictating the direction of future steps. To simulate persistent motion, one must resort to the emerging field of fractal statistics.

In the following, traditional particle tracking models and their properties are briefly reviewed before discussing the practical generation of fractional Brownian motions (FBMs) and their associated fractal and diffusion characteristics. The diffusion of a contaminant release in a numerical example using both a traditional particle tracking model and one based on FBMs is then compared.

## 2. TRADITIONAL RANDOM WALK MODELS

Traditional random walk models of diffusion release a large number of massless, marked particles into the flow field and allow them to diffuse by taking random steps in each spatial direction.[5] This diffusion is combined with the mean flow advection, calculated from a knowledge of the mean flow velocity vector field. The random steps taken by traditional models are usually obtained from either a Gaussian probability distribution or, in an attempt to reduce computing time, a simpler constant or delta function distribution. These simpler distributions produce accurate results for large time scales as they give good approximations to Brownian motion owing to the central limit theorem. There is, however, one fundamental drawback with the traditional random walk technique. That is, as long as the steps are statistically independent from one instance in time to the next, then, regardless of the form of the probability distribution from which the random steps are taken, only Fickian diffusion can be produced. Therefore, if a large enough number of particles are used in a particle-tracking model, the resultant standard deviation $\sigma_c$ of the particle cloud scales with the square root of time since release,[12] i.e.

$$\sigma_c = \sqrt{(2Dt)}, \tag{1}$$

where $D$ is the diffusion coefficient. In practice, diffusion coefficients may be found for each spatial direction in the flow field. Hence a discretized approximation to a Brownian motion in each spatial direction, $B(t_i)$, may be produced at discrete times $t_i = i\Delta t$, (where $i$ is an integer and $\Delta t$ is the time step) by summing a series of random steps taken from a Gaussian distribution, $R(t_i)$, i.e.

$$B(t_i) = \sum_{j=1}^{i} R(t_j). \tag{2}$$

To simulate the required diffusion, a standard deviation $\sigma_p$ of the random particle steps $R(t_i)$ is employed, where,

$$\sigma_p = \sqrt{(2D\Delta t)}. \tag{3}$$

Hence after $N$ steps the standard deviation of the resultant cloud is given simply by

$$\sigma_c = \sigma_p N^{1/2}. \tag{4}$$

As mentioned above, $R(t_i)$ may be a simpler distribution. If this is the case equations (3) and (4) still hold, however, the shape of the diffusing cloud over short times will not be Gaussian. The shape will change towards Gaussian over sufficiently large times—a manifestation of the central limit theorem.

## 3. FRACTIONAL BROWNIAN MOTION AND THE FRACTAL STRUCTURE OF DIFFUSING PARTICLE PATHS

The Brownian motion of Section 2 is a special member of the larger family of fractional Brownian motions.[13,14] (For reasons of clarity in the discussion below, Brownian motion as discussed above will be referred to as regular Brownian motion.) As with regular Brownian motion, fractional Brownian motion is generated by summing a series of random steps taken from a Gaussian distribution. This time, however, the summation is weighted over the preceding Brownian steps. This generates long-time power-law correlations within the resulting motion. In the limit the FBM is defined as

$$B_H(t) = \frac{1}{\Gamma(H+\frac{1}{2})} \int_{-\infty}^{t} (t-t')^{H-1/2} R(t')\,\mathrm{d}t', \tag{5}$$

where $B_H(t)$ is the fractional Brownian motion at time $t$, $R(t)$ is a continuous white noise function, $H$ is the Hurst[15,16] scaling exponent and $\Gamma$ is the gamma function. The fractional integral of equation (5) is not practically useful owing to the requirement to integrate back to negative infinity in order to realize the FBM at time $t$. A further problem with the above definition is that it diverges as $t'$ approaches $-\infty$. To use such a model, it is necessary to specify an FBM which goes through the origin, i.e. $B_H(t) = 0$ at $t = 0$. This can be achieved by subtracting the FBM at time $t = 0$, i.e.

$$B_H(0) = \frac{1}{\Gamma(H+\frac{1}{2})} \int_{-\infty}^{0} (0-t')^{H-1/2} R(t')\,\mathrm{d}t, \tag{6}$$

from the original definition, (5). Rearranging the terms gives

$$B_H(t) - B_H(0) = \frac{1}{\Gamma(H+\frac{1}{2})} \left( \int_{-\infty}^{0} [(t-t')^{H-1/2} - (-t')^{H-1/2}] R(t')\,\mathrm{d}t' - \int_{0}^{t} (t-t')^{H-1/2} R(t')\,\mathrm{d}t' \right). \tag{7}$$

The problem still remains of having to integrate back to negative infinity to correctly define the FBM. This can be overcome by using a finite memory leading to a discretised approximation to an FBM, based on (7), defined as

$$B_H(t_i) = \frac{1}{\Gamma(H+\frac{1}{2})} \left( \sum_{j=i-M}^{0} [(i-j)^{H-1/2} - (-j)^{H-1/2}] R(t_j) + \sum_{j=1}^{i} (i-j)^{H-1/2} R(t_j) \right), \tag{8}$$

where $B_H(t_i)$ is the $i$th discrete approximation to the FBM at time $t_i$; $M\Delta t$ is the limited temporal memory used in the approximation of the FBM; and $R(t_i)$ are random steps discretely sampled from a Gaussian probability distribution. There is an obvious computational cost involved in using the FBM of (8) rather than the regular Brownian motion of (2), as each step taken in the FBM model requires the summation of $M$ previous steps. Equation (8) reduces to the regular Brownian motion of (2) when $H = 0{\cdot}5$. Depending on the value of the Hurst exponent, the trace generated from (8) will be antipersistant ($H < 0{\cdot}5$), neutrally persistent ($H = 0{\cdot}5$) or persistent ($H > 0{\cdot}5$).[17] Here we concentrate on persistent FBMs which lead to non-Fickian scaling with characteristics similar to superdiffusing particles in turbulent fluids. The paths of particles undergoing fractional Brownian motion in two- and three-dimensional flow fields may be generated using (8) to calculate the temporal evolution of each spatial co-ordinate.[18]

Figure 1 contains trajectories in the plane of two particles, one undergoing regular Brownian motion (i.e. $H = 0{\cdot}5$) and the other an FBM with Hurst exponent equal to 0·75. For simplicity, both the diffusion coefficient and the time step are set to unity in each case and 1000 steps are plotted. In the figure, equations (2) and (8) respectively are used to produce the spatial co-ordinates of the trajectories in the plane. A comparison of the two figures shows up the persistent quality of the FBM trajectory, which Mandelbrot[19] described as *an appropriately intense tendency but not an obligation to avoid self-intersection*.

Extensive studies by Osborne *et al.*[8] and Sanderson and Booth[10] found that the trajectories of satellite-tracked ocean surface drifters may be described as persistent fractional Brownian motions

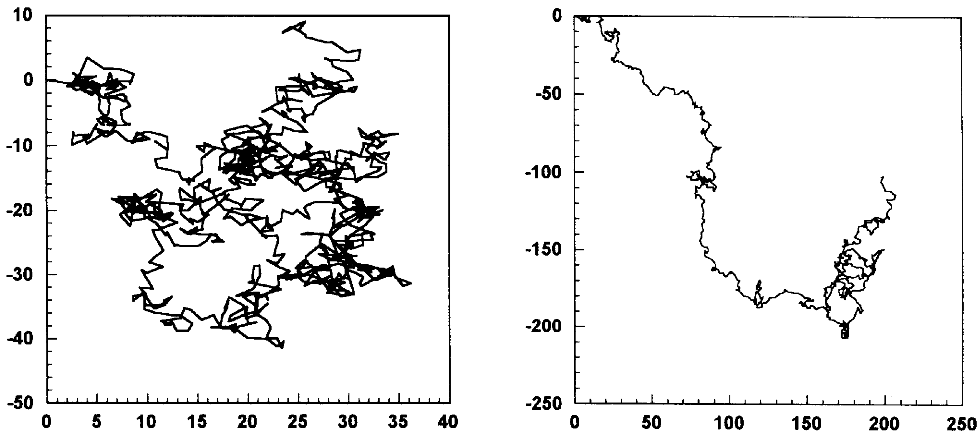


Figure 1. Regular and fractional Brownian motions

with non-Fickian scaling properties. The studies were conducted in two separate regions of the globe, the Northeast Atlantic and the Kurisho extension respectively, and yielded general agreement with the Hurst exponents found, which all lay around $0{\cdot}79 \pm 0{\cdot}07$. In addition to the Hurst exponent, both studies characterized the fractional Brownian motions of the trajectories in terms of their fractal geometric properties through the fractal dimension $\delta$. The fractal dimension is the more natural measure with which to characterize fractional Brownian motions, which are random fractals with statistical self-similarity at all scales. The fractal dimension is an indication of the ability of the FBM trajectory to fill up the space in which it exists and is related to the Hurst exponent through the expression[20]

$$\delta = \min[1/H, 2]. \tag{9}$$

Persistent FBMs in the plane are more likely to wander off than remain to fill up the plane densely, hence their fractal dimension lies in the range $1 < \delta < 2$. That is, they have a fractal dimension less than the Euclidean plane in which they exist.[21,22]

The standard deviation of a diffusing cloud of FBM particles scales with time raised to the power of the Hurst exponent $H$, giving a fractal diffusion relationship

$$\sigma_c = (2Dt)^H, \tag{10}$$

where again $D$ is the diffusion coefficient. Note that both a diffusion coefficient and a scaling exponent are required to define fractal diffusion, as the exponent of $\frac{1}{2}$ of regular Brownian motion has been replaced with the more general Hurst exponent $H$ of fractional Brownian motion, where $0 < H < 1$. Equation (10) leads to expected variances of 31·6 and 177·8 respectively for the simulated trajectories in Figures 1(a) and 1(b). The spatial extents of the trajectories in the figures are of the order of these numbers.

## 4. A NUMERICAL EXAMPLE: SURFACE DIFFUSION IN AN OPEN BAY

In this section the new method is applied to the modelling of two-dimensional surface diffusion in the coastal zone. An idealized open bay with a main-flow-driven recirculation pattern is employed. The model includes only main flow advection and turbulent diffusion generated by the FBM model, tidal and other diffusion mechanisms are ignored[23,24]. A Hurst exponent of 0·75 is employed in both spatial directions for simplicity. In reality the scaling exponent in the coastal zone can be complex.[25]

The test case developed was based on an idealized coastal bay that sloped from deep water in the west to a shallow bay in the east. The main channel has a depth of 50 m over the first 500 m then shallows to 10 m at the eastern coastline. Figure 2 shows the uniform grid, with cells 100 m by 100 m, along with the contour plot of the bay.

A surface velocity distribution was obtained from a layered two dimensional hydrodynamic model. In the model a constant inflow of 0·5 m/s was set at the northern boundary. In Figure 3 the velocity vector plot for the surface layer is shown. Once the velocity field had been generated, four test cases (two pairs) were selected:

(i) a release in the bay, using regular Brownian motion
(ii) a release in the bay, using fractional Brownian motion with a Hurst exponent of 0·75
(iii) a release upstream of the bay, using regular Brownian motion
(iv) a release upstream of the bay, using fractional Brownian motion with a Hurst exponent of 0·75.

For all cases the diffusion coefficient was set at $D = 0{\cdot}01\ \mathrm{m}^2/\mathrm{s}^{-1}$ in both spatial directions. Owing to the computational intensity of the FBM technique, only 400 particles were released in each test case. Generally larger numbers of particles (of the order of 10,000s) are used in numerical simulations; however, this smaller number was found adequate to illustrate the problem herein. The particles moved through the computational grid, advected by the mean advection velocity, found from bilinear interpolation of the four velocity vectors at the corners of the grid cell, and diffused by taking random steps according to either (2) or (8). The results from these test cases are illustrated in Figures 5–8.

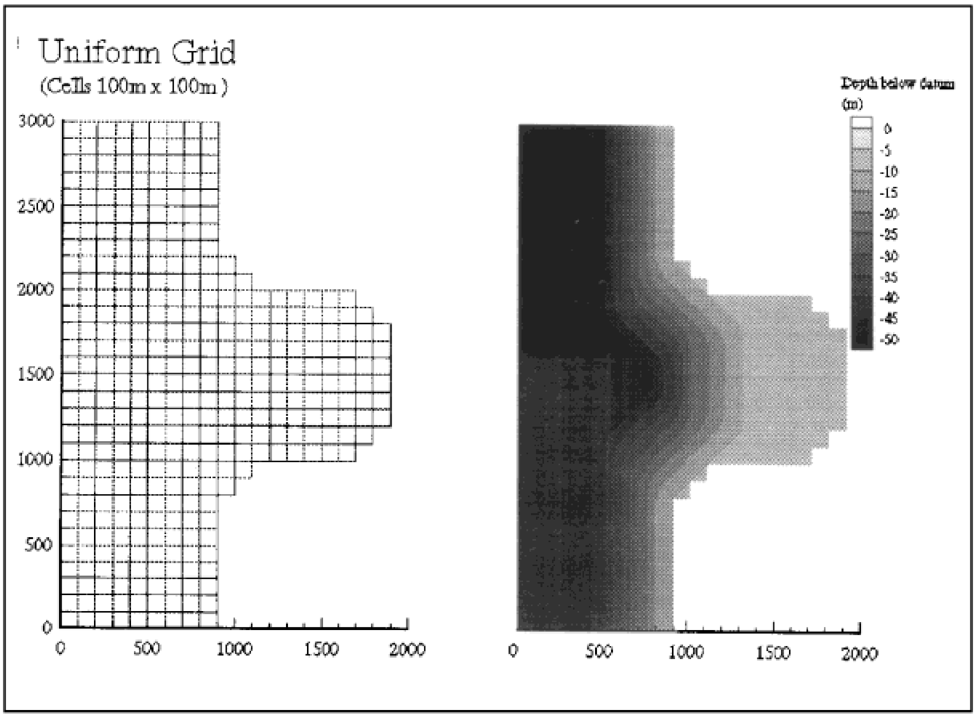


Figure 2. Simulation geometry: uniform grid and contour plot of bottom surface topography

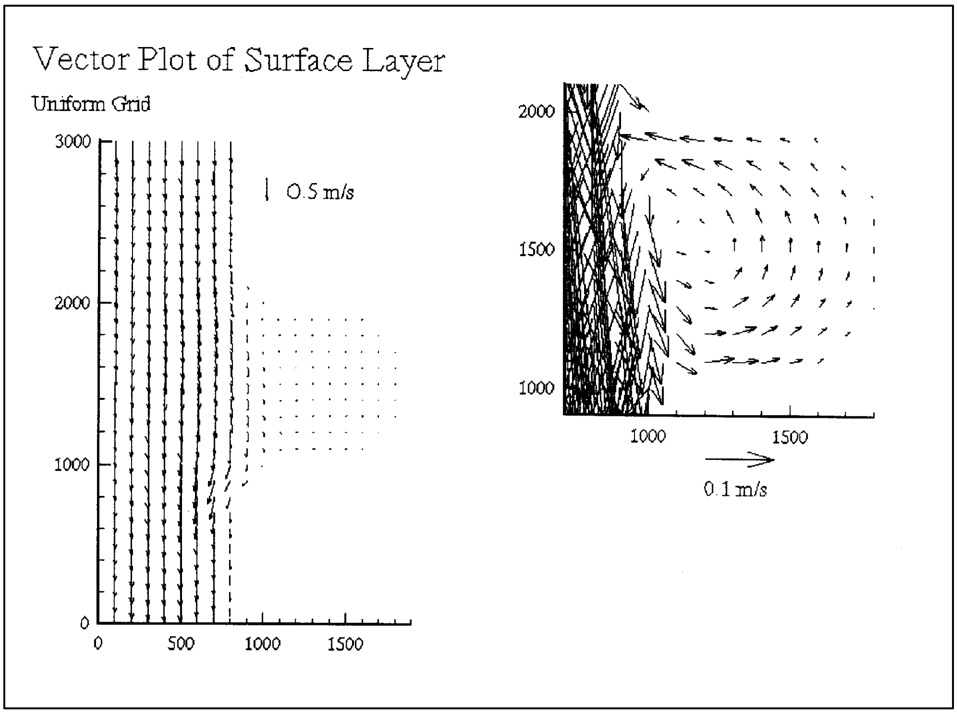


Figure 3. Velocity vector field for surface layer

Before discussing these figures, it is useful to look at Figure 4, which contains a diffusion-only plot of 400 marked particles 6 h after release, i.e. without mean flow advection. The standard deviations of the resultant clouds in Figure 4 are 20·8 and 94·8 respectively—almost a fivefold increase in the diffusion after 6 h of simulation.

Figures 5 and 6 contain the diffusion of the particle cloud released from grid position (1200, 1700) at time $t = 0$. In Figure 5 the particles in the cloud follow regular Brownian paths ($H = 0{\cdot}5$). The subsequent spreading of the particle cloud can be followed, in 2 h increments, until 12 h after release. The entrapment of the particle cloud within the recirculatory bay flow can be seen. Figure 6 contains the particle cloud released from the same location as for Figure 5, but this time the particles follow fractional Brownian paths with $H = 0{\cdot}75$. There is a noticeable increase in the spreading rate of the cloud, which in physical terms would mean a sharper reduction in contaminant concentration with time. This in turn has important implications for the predicted toxicity levels to a physiologically safe level in the environment. In addition, owing to the increased spreading of the FBM particle cloud, a noticeable part of it has escaped the bay area and is transported downstream. This again is important, whereby a variation in the Hurst exponent can lead to an area of the flow field being affected by a contaminant cloud which is not picked up by the regular Brownian motion models used in practice.

Figures 7 and 8 contain the diffusion of the particle cloud released at grid position (850, 2500) which is in the main flow outside the bay recirculation zone. These figures essentially reconfirm the behaviour observed in Figures 5 and 6. In Figure 7 the regular Brownian particle cloud remains fairly compact as it is advected by the main flow at the boundary of the recirculation zone. Most of the cloud is advected past the bay region and contacts with the downstream shoreline. A small part of the cloud is advected into the bay region, again staying close to the shore. In Figure 8 the evolution of the

 

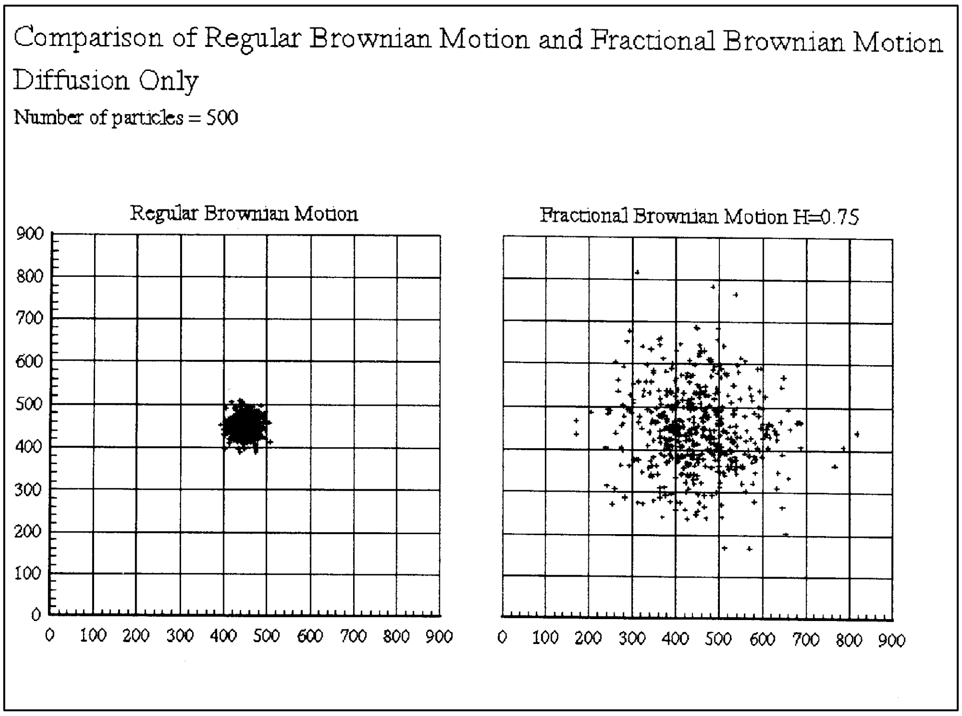


Figure 4. Diffusion without convection of particle cloud undergoing regular Brownian motion ($H = 0{\cdot}5$) and fractional Brownian motion ($H = 0{\cdot}75$) 6 h after release; $D = 0{\cdot}01\ \mathrm{m}^2\,\mathrm{s}^{-1}$

FBM cloud released in the main flow region is shown. Again a much faster spreading of the cloud is evident from the figure, which leads to more particles moving both closer to the slower-moving flow at the upstream shoreline and into the faster-moving main flow, resulting in an attenuated contaminant plume after 2 h compared with the corresponding plot in Figure 7. In addition, the greater spreading forces more of the cloud into the bay area; however, it also leads to a more even concentration distribution within the bay, as the particles are not confined to the shoreline as was the case with $H = 0{\cdot}5$. Thus an increase in pollution entrapment in the bay region does not necessarily lead to an increase in contamination of the bay shoreline itself.

## 5. CONCLUDING REMARKS

A simple method has been described for the generation of non-Fickian diffusion in a particle-tracking diffusion model by employing fractional Brownian motions. A practical algorithm for their generation is given in the form of (8), which is an improvement on the method suggested by Addison.[17] The method allows for diffusion, as characterized by a typical length scale in the diffusing cloud, scaling with time raised to the power of $H$, the Hurst exponent, where $0 < H < 1$. The technique has been illustrated in a numerical example of surface diffusion in the coastal zone, where the exponential scaling of the diffusion becomes an important factor in determining future locations and concentrations of the contaminant cloud. Particle-tracking models which incorporate fractional Brownian motions will provide the numerical modeller with an enhanced tool for the simulation of pollutant dispersal by providing more flexibility to account for the non-linear scalings of diffusion in the environment.

 

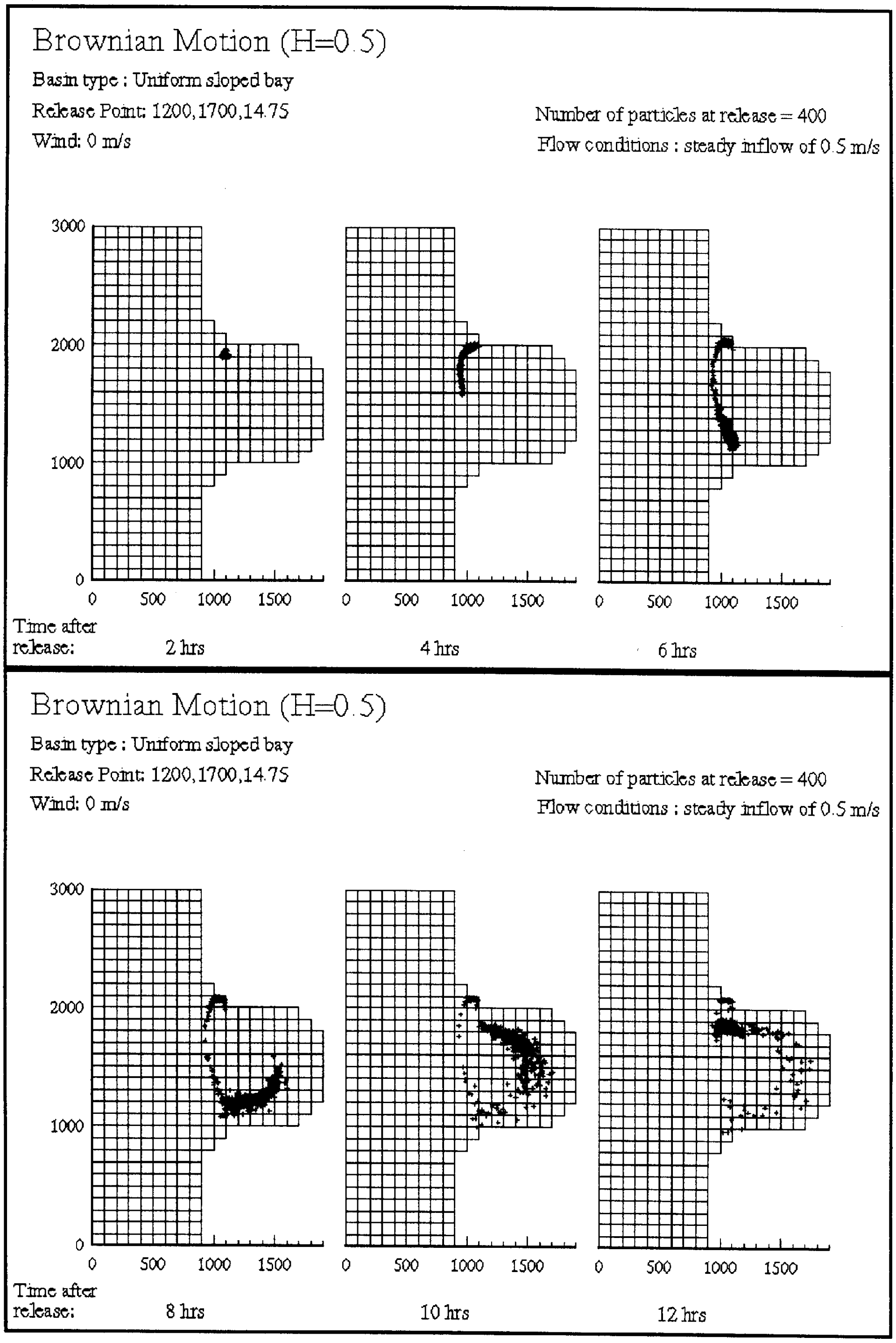


Figure 5. Release in bay—regular Brownian motion

 

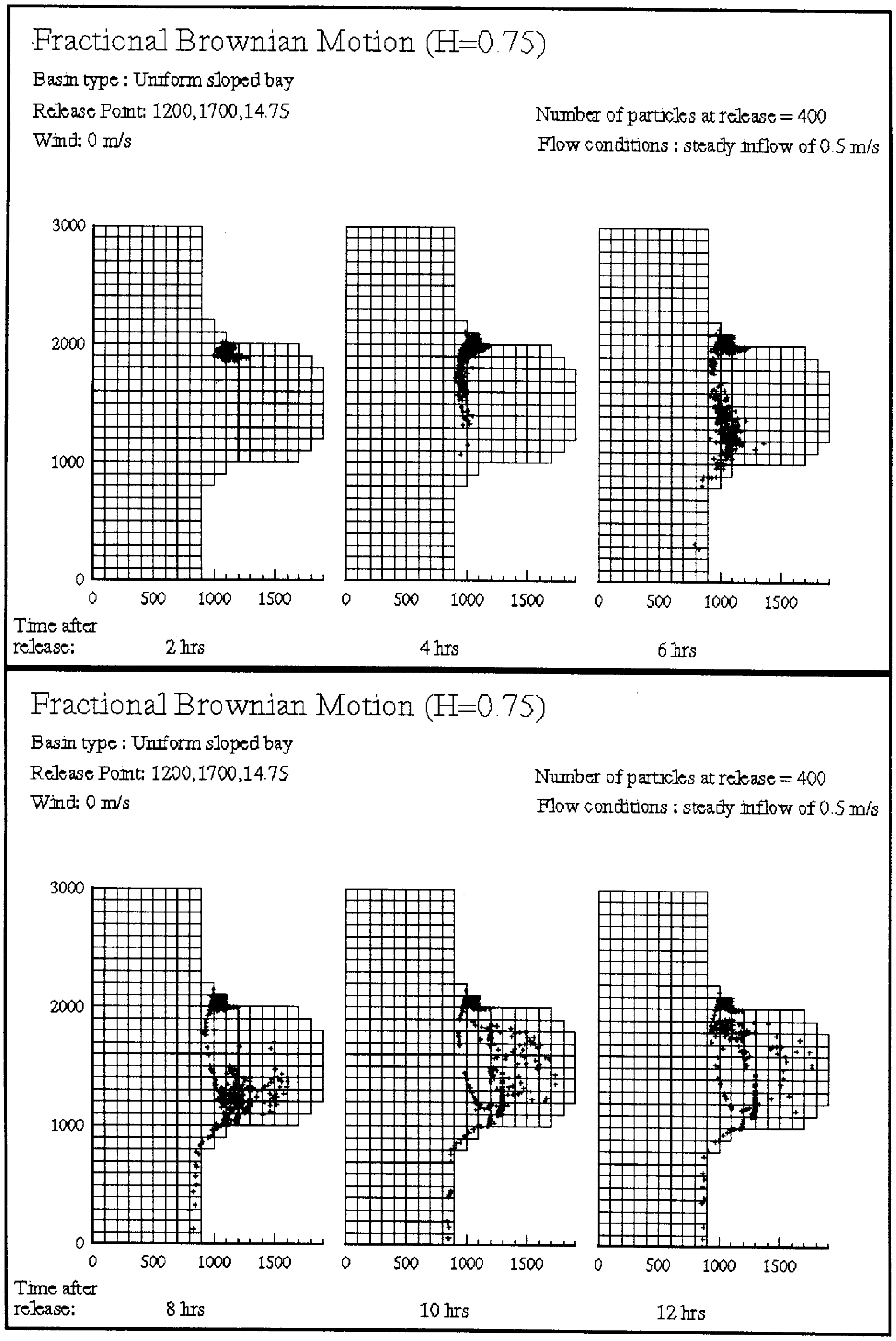


Figure 6. Release in bay—fractional Brownian motion with $H = 0{\cdot}75$

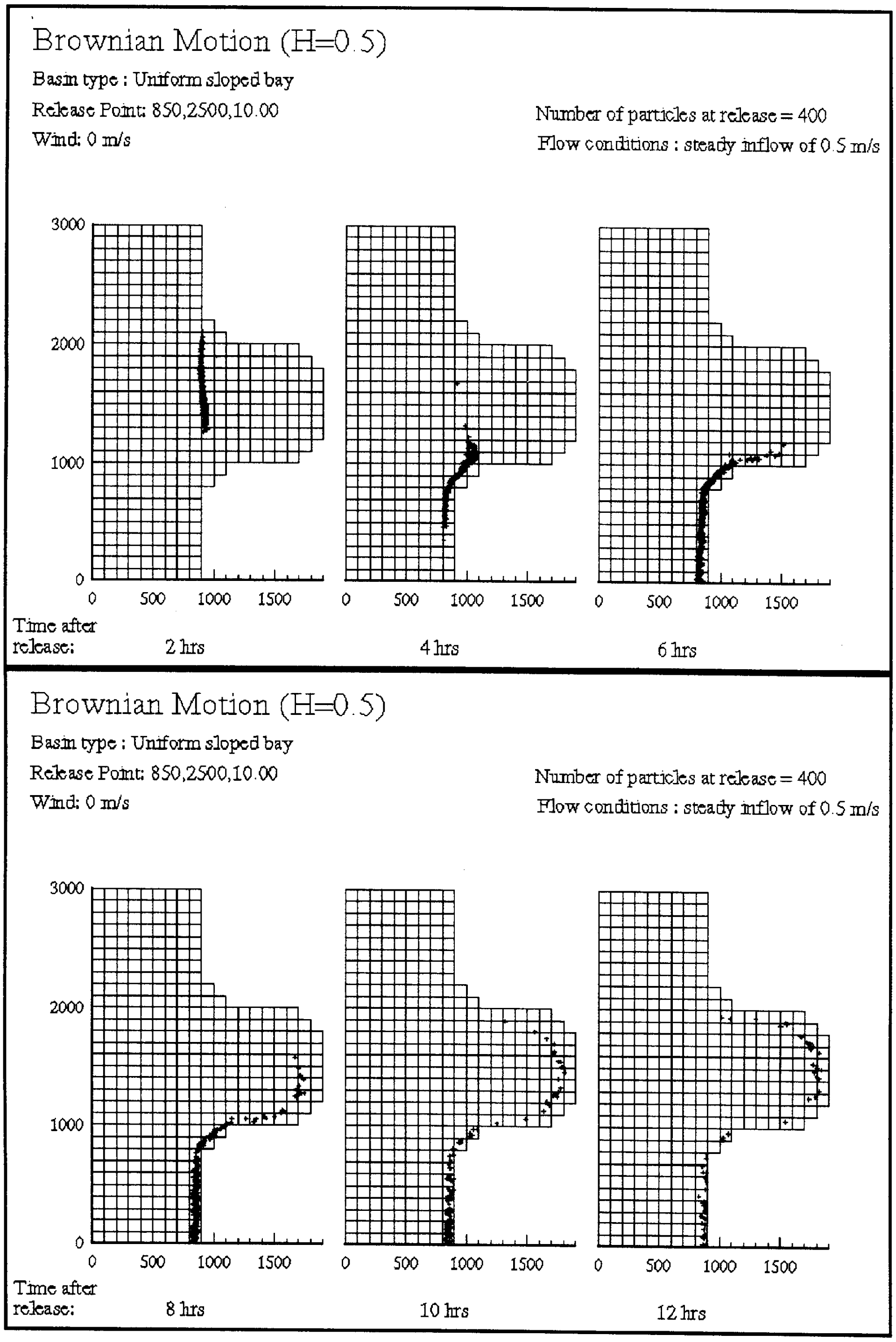


Figure 7. Release upstream of bay—regular Brownian motion

 

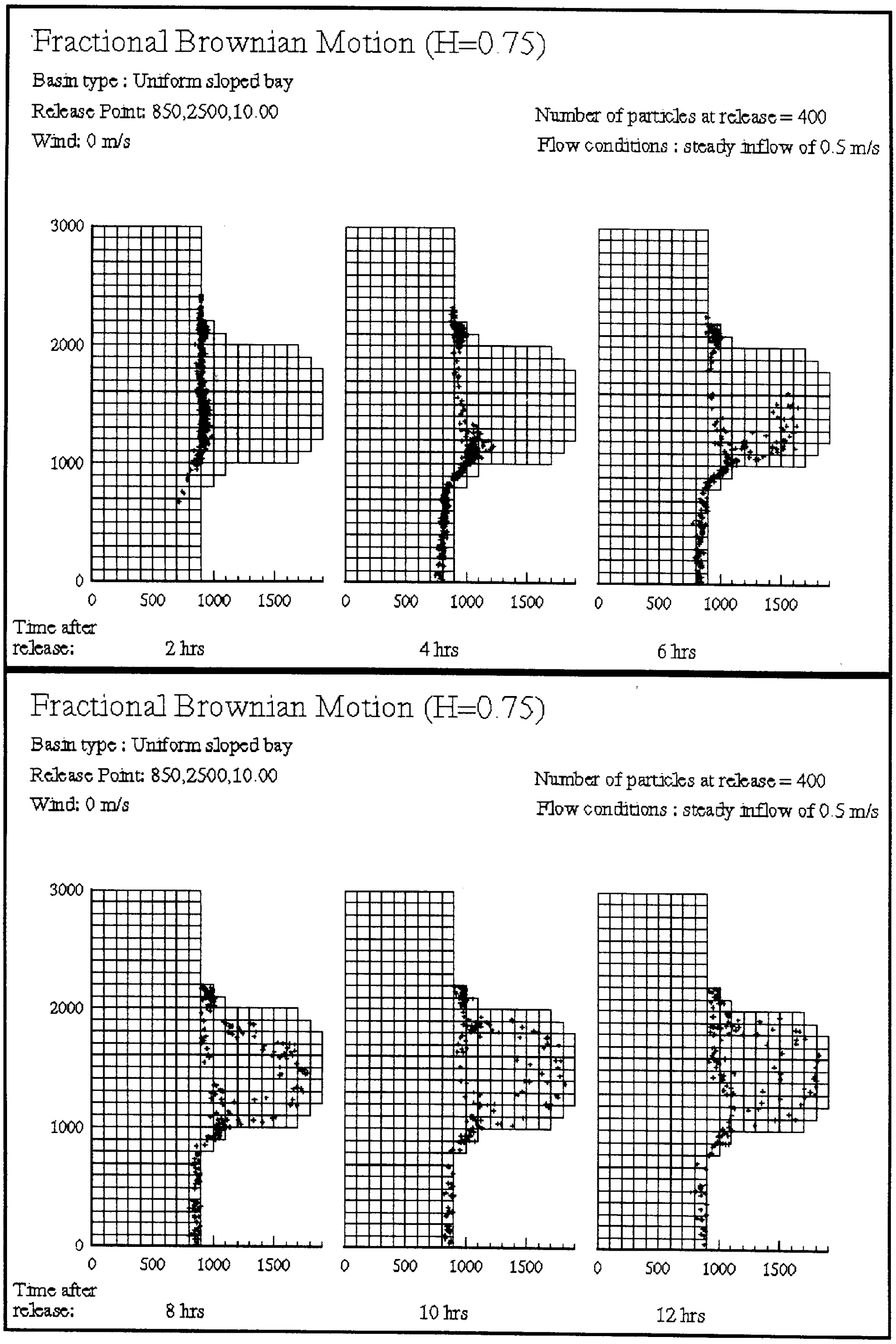


Figure 8. Release upstream of bay—fractional Brownian motion with $H = 0{\cdot}75$

It is a simple task to extend the technique to model three-dimensional non-Fickian diffusion should theoretical and/or experimental advances support its use.[26] Subsequent work aims to develop the computational efficiency of the model[27,28] and use accelerated fractional Brownian motion[10] to model two-particle dispersion, where patch variance may grow at a rate with exponent greater than two.[29]

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