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Coloured noise for dispersion of contaminants in shallow waters

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Abstract

In this article, we explore the application of a set of stochastic differential equations called particle model in simulating the advection and diffusion of pollutants in shallow waters. The Fokker–Planck equation associated with this set of stochastic differential equations is interpreted as an advection–diffusion equation. This enables us to derive an underlying particle model that is exactly consistent with the advection–diffusion equation. Still, neither the advection–diffusion equation nor the related traditional particle model accurately takes into account the short-term spreading behaviour of particles. To improve the behaviour of the model shortly after the deployment of contaminants, a particle model forced by a coloured noise process is developed in this article. The use of coloured noise as a driving force unlike Brownian motion, enables to us to take into account the short-term correlated turbulent fluid flow velocity of the particles. Furthermore, it is shown that for long-term simulations of the dispersion of particles, both the particle due to Brownian motion and the particle model due to coloured noise are consistent with the advection–diffusion equation.
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1. Introduction

The increasingly awareness in most societies of issues such as water and air pollution has lead to the need for ways to alleviate or reverse the situation. The use of mathematical models is relevant in the simulations and prediction of pollutants transport. Thus, a significant development of various mathematical models for advection and dispersion of pollution in shallow waters have been developed [1–4], for example. These model are used for predictions of pollutant dispersion as well as for plans to improve water quality in shallow waters such as in rivers and coastal water. Of the available methods, particle models are gaining popularity [5]. This is because they are easy to implement, can be used for a wide range of applications [4]. On the other hand, there are well-known intricacies associated with the finite difference schemes used for approximating the

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advection–diffusion equations. Moreover, the use of particle tracking models can provide valuable information to assist in problem analysis, optimisation and environmental modelling. However, most of these particle models use Brownian motion force for simulating the diffusion/dispersion of particles is shallow waters [1,6,7]. Such models consider that particles move according to a simple random walk and consequently have independent increment [8,5]. These models are consistent with the well-known advection–diffusion models for transport of pollutants in shallow waters. However, it is well known that the advection–diffusion equation describes the dispersion of particles in turbulent fluid flow accurately if the diffusing cloud of contaminants has been in the flow longer than a certain Lagrangian time scale and has spread to cover a distance that is larger in size than the largest scale of the turbulent fluid flow [6]. The Lagrangian time scale (T_L) is a measure of how long it takes before a particle loses memory of its initial turbulent velocity. In reality, however, there exists short-term correlation in a variety of hydraulic engineering problems including coastal waters and subsurface diffusion [4]. Therefore, both the particle model due to Brownian force and the advection–diffusion model are unable to accurately describe the short time scale correlated behaviour which is available in real turbulent flows at sub-Lagrangian time. Thus, this papers instead we develop a model which is forced by coloured noise. This way, the particle model takes correctly into account the diffusion processes over short time scales when the eddy (turbulent) diffusion is less than the molecular diffusion. The inclusion of several parameters in the coloured noise process allows for a better match between the auto-covariance of the model and the underlying physical processes. In addition, the particle model forced by coloured noise model has been developed in such a way that the coloured noise process approximates Brownian motion over large time periods. The advection–diffusion equation can also be improved to account for the short-term correlation behaviours. The resulting Eulerian model is equivalent to the developed particle model for small scale time. In this article, we implement both the classical particle model and the particle model due to coloured noise. Because they are relatively much easier [3] than the numerical implementation of the equivalent Eulerian transport model. Note that the random flight model takes into account the correlation behaviour of particle's position at time t and its initial location. The correlation between the two particles is not taken into account because we use a one-particle model [6]. One-particle models describe transport of a single particle. By performing experiments with many different particles, an ensemble mean concentration can be obtained by averaging the results of all individual particles in the experiments. The resulting average concentration value is an important quantity as far as the prediction processes is concerned. The remainder of this paper is organised as follows, in Section 2 we briefly introduce the traditional particle model. Section 4 introduces coloured noise processes. Explanations of the techniques for modelling dispersing pollutants are outlined in Section 5. The general random flight model is developed in Section 5.1. The analysis of spreading properties of a cloud of contaminants such as the variance is done in Section 6. Several numerical experiments are carried out in Section 8. Finally, in Section 10 both the traditional particle model and the particle model due to coloured noise are applied to predict the dispersion of pollutants in the Dutch coastal waters.

2. Particle model due to Brownian motion force for dispersion of pollutants in shallow waters

The position of particles in water at time t, is designated by $(X(t), Y(t))$. Different random locations of the particle are described with the aid of stochastic differential equation. The integration of the movements of the particle in water is done in two steps. A deterministic step consisting of velocity field of water and a random step known as diffusion modelled by the stochastic process [1];

$$\mathrm{d}X(t) \overset{\text{Itô}}{=} \left[U + \frac{D}{H}\frac{\partial H}{\partial x} + \frac{\partial D}{\partial x}\right]\mathrm{d}t + \sqrt{2D}\,\mathrm{d}B_1(t), \quad X(0) = x_0, \tag{1}$$

$$\mathrm{d}Y(t) \overset{\text{Itô}}{=} \left[V + \frac{D}{H}\frac{\partial H}{\partial y} + \frac{\partial D}{\partial y}\right]\mathrm{d}t + \sqrt{2D}\,\mathrm{d}B_2(t), \quad Y(0) = y_0. \tag{2}$$

Here D is the dispersion coefficient in m^2/s; $U(x,y,t), V(x,y,t)$ are the averaged flow velocities (m/s) in respectively x, y directions; $H(x,y,t)$ is the total depth in m at location (x,y), and $\mathrm{d}B(t)$ is a Brownian motion with mean $(0,0)^T$ and $\mathbb{E}[\mathrm{d}B_1(t)\mathrm{d}B_2(t)^T] = I\,\mathrm{d}t$ where I is a 2×2 identity matrix [9]. Note that the advective part of the particle model Eqs. (1)–(2) is not only containing the averaged water flow velocities but also spatial

variations of the diffusion coefficient and the averaged depth. This correction term makes sure that particles are not allowed to be accumulated in regions of low diffusivity as demonstrated by (see e.g., [7,3]). At closed boundaries particle bending is done by halving the time step sizes until the particle no longer crosses closed boundary. As a result there is no loss of mass through such boundaries. The position $(X(t), Y(t))$ process is Markovian and the evolution of its probability density function $(p(x,y,t))$, is described by an advection–diffusion type of the partial differential equation known as the Fokker–Planck equation (see e.g.,[8])

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left(\left[U + \frac{D}{H}\frac{\partial H}{\partial x} + \frac{\partial D}{\partial x}\right]p\right) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(2Dp) + \frac{1}{2}\frac{\partial^2}{\partial y^2}(2Dp) - \frac{\partial}{\partial y}\left(\left[V + \frac{D}{H}\frac{\partial H}{\partial y} + \frac{\partial D}{\partial y}\right]p\right). \tag{3}$$

The initial spreading of a cloud of particles is very small and its distribution can be modelled using a Dirac delta function.

$$p(x,y,t_0) = \delta(x - x_0)\delta(y - y_0). \tag{4}$$

This is physically a way of representing a larger concentration or number of particles into an infinitely small space (see e.g., [8,6]).The probability density function of particles at a certain location is an exposition of the concentration at that location [1,6], therefore particle concentration $C(x,y,t)$ can be related to the probability density function $p(x,y,t)$:

$$C(x,y,t) = p(x,y,t)/H(x,y,t). \tag{5}$$

By substituting this equation into Fokker–Planck Eq. (3), the following vertically integrated advection–diffusion equation can be derived:

$$\frac{\partial(HC)}{\partial t} = -\frac{\partial(HUC)}{\partial x} - \frac{\partial(HVC)}{\partial y} + \frac{\partial}{\partial x}\left(DH\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(DH\frac{\partial C}{\partial y}\right). \tag{6}$$

An initial condition for the concentration can subsequently be obtained by substituting Eq. (4) into Eq. (5). Where U,V are the flow fields along x and y directions, respectively.H is the total water depth, D is the dispersion coefficient. By interpreting the Fokker–Planck equation (3) as the vertically integrated advection–diffusion equation makes the particle model in Eqs. (1)–(2) to be consistent with the well-known advection–diffusion Eq. (6) as shown by [1]. The inputs such as flow velocities, water depth and so forth required by the particle transport model are computed by the hydrodynamic model known as WAQUA [10].This is briefly described in the following section.

3. Shallow water flow equations

In order for particle models to describe transport problems in shallow waters, the inputs such as water flow velocities $[U(x,y,t), V(x,y,t)]^T$, water levels ξ, water depths $H(x,y,t)$ and so forth are required. In our application, the inputs are often computed by the hydrodynamic model (WAQUA), which can solve the depth-averaged shallow water equations or 3 dimensional shallow water [10]. The inputs are assumed to satisfy the shallow water equations [1]. The momentum equations are represented by the following equations:

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y} + g\frac{\partial \xi}{\partial x} - fV + g\frac{U(U^2+V^2)^{\frac{1}{2}}}{(C_z)^2 H} = 0, \tag{7}$$

$$\frac{\partial V}{\partial t} + U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y} + g\frac{\partial \xi}{\partial y} + fU + g\frac{V(U^2+V^2)^{\frac{1}{2}}}{(C_z)^2 H} = 0. \tag{8}$$

The velocity is uniform over the vertical, therefore, for that reason, the rise and fall of free surface is given by equations of conservation of mass called the continuity equation:

$$\frac{\partial H}{\partial t} + \frac{\partial(UH)}{\partial x} + \frac{\partial(VH)}{\partial y} = 0, \tag{9}$$

where
$H = h + \xi$ is the total depth
ξ is the water-level with respect to a reference
h depth of the water with respect to a reference
C_z bottom friction coefficient (Chezy coefficient)
g acceleration of gravity
f Coriolis parameter.

The shallow water equations are entirely described by Eqs. (7)–(9), provided the closed and open boundary conditions and initial fields are given [1].

4. Coloured noise processes

In this part, coloured noise forces are introduced and represent the stochastic velocities of the particles, induced by turbulent fluid flow. It is assumed that this turbulence is isotropic and that the coloured noise processes are stationary and completely described by their zero mean and Lagrangian auto-covariance function.

4.1. The scalar exponential coloured noise process

Let the linear stochastic differential equation that models the dynamics of a stochastic velocity of the particle be given by

$$\mathrm{d}u_1(t) = -\frac{1}{T_L}u_1(t)\mathrm{d}t + \alpha_1 \mathrm{d}B(t), \tag{10}$$

$$u_1(t) = u_0 \mathrm{e}^{\frac{-t}{T_L}} + \alpha_1 \int_0^t \mathrm{e}^{-\frac{(t-s)}{T_L}} \mathrm{d}B(s), \tag{11}$$

where $\alpha_1 > 0$ is constant, and T_L is a Lagrangian time scale. For $t > s$ it can be shown [8], that the scalar exponential coloured noise process in Eq. (11) has mean, variance and Lagrangian auto-covariance of, respectively,

$$\mathbb{E}[u_1(t)] = u_0 \mathrm{e}^{\frac{-t}{T_L}}, \quad \mathrm{Var}[u_1(t)] = \frac{\alpha_1^2 T_L}{2}\left(1 - \mathrm{e}^{-\frac{2t}{T_L}}\right), \quad \mathrm{Cov}[u_1(t), u_1(s)] = \frac{\alpha_1^2 T_L}{2}\mathrm{e}^{-\frac{|t-s|}{T_L}}. \tag{12}$$

4.2. The general vector coloured noise force

The general vector form of a linear stochastic differential equation for coloured noise processes [8,11] is given by

$$\mathrm{d}\mathbf{u}(t) = F\mathbf{u}(t)\mathrm{d}t + G(t)\mathrm{d}B(t), \quad \mathrm{d}\mathbf{v}(t) = F\mathbf{v}(t)\mathrm{d}t + G(t)\mathrm{d}B(t), \tag{13}$$

where $\mathbf{u}(t)$ and $\mathbf{v}(t)$ are vectors of length n, F and G are $n \times n$ respectively $n \times m$ matrix functions in time and $\{B(t); t \geqslant 0\}$ is an m-vector Brownian process with $\mathbb{E}[\mathrm{d}B(t)\mathrm{d}B(t)^T] = Q(t)\mathrm{d}t$. In this article, we extend a special case of the Ornstein–Uhlenbeck process [12,11], and repeatedly integrate it to obtain the coloured noise forcing along the x and y directions:

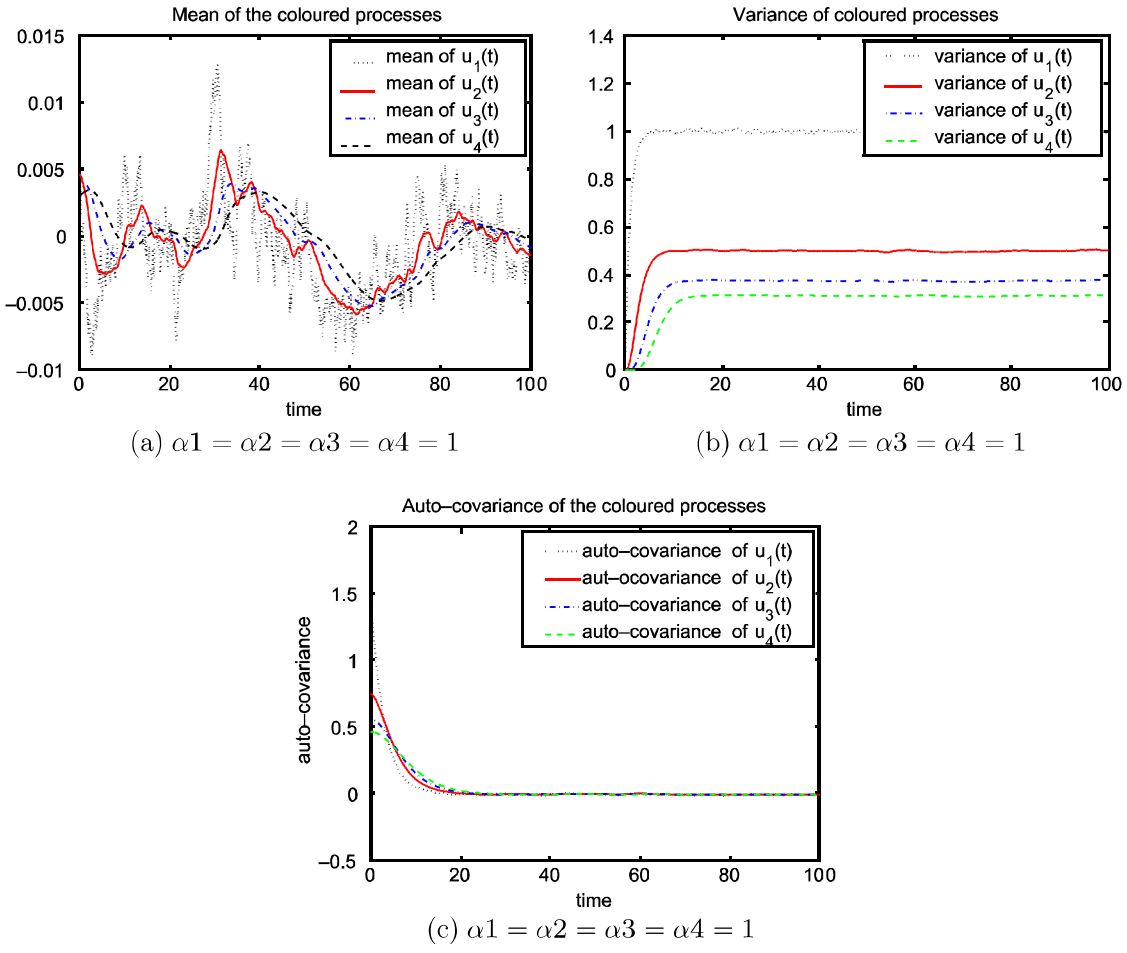
$$\begin{aligned}
\mathrm{d}u_1(t) &= -\tfrac{1}{T_L}u_1(t)\mathrm{d}t + \alpha_1\mathrm{d}B(t), & \mathrm{d}v_1(t) &= -\tfrac{1}{T_L}v_1(t)\mathrm{d}t + \alpha_1\mathrm{d}B(t),\\
\mathrm{d}u_2(t) &= -\tfrac{1}{T_L}u_2(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_2 u_1(t)\mathrm{d}t, & \mathrm{d}v_2(t) &= -\tfrac{1}{T_L}v_2(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_2 v_1(t)\mathrm{d}t,\\
\mathrm{d}u_3(t) &= -\tfrac{1}{T_L}u_3(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_3 u_2(t)\mathrm{d}t, & \mathrm{d}v_3(t) &= -\tfrac{1}{T_L}v_3(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_3 v_2(t)\mathrm{d}t,\\
\mathrm{d}u_4(t) &= -\tfrac{1}{T_L}u_4(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_4 u_3(t)\mathrm{d}t, & \mathrm{d}v_4(t) &= -\tfrac{1}{T_L}v_4(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_4 v_3(t)\mathrm{d}t,\\
\vdots \quad &= \quad \vdots & \vdots \quad &= \quad \vdots\\
\mathrm{d}u_n(t) &= -\tfrac{1}{T_L}u_n(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_n u_{n-1}(t)\mathrm{d}t, & \mathrm{d}v_n(t) &= -\tfrac{1}{T_L}v_n(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_n v_{n-1}(t)\mathrm{d}t.
\end{aligned} \tag{14}$$

By doing this, a Lagrangian auto-covariance of the velocity processes is modelled more accurately and becomes possible to take into account the characteristics of an isotropic homogeneous turbulent fluid flow. The vector Langevin equation (14) generates a stationary, zero-mean, correlated Gaussian process denoted by $(u_n(t), v_n(t))$. The Lagrangian time scale T_L indicates the time over which the process remains significantly correlated in time. The linear system in Eq. (14), is the same in the Itô and the Stratonovich sense because the diffusion function is not a function of state but only of time. In order to get more accurate results we integrate the stochastic differential equation that is driven by the coloured noise processes by the Heun scheme (see e.g., [13,2,9]).

The main purpose of this article is the application of coloured noise forcing in the dispersion of a cloud of contaminants so as to improve the short-term behaviour of the model while leaving the long-term behaviour unchanged. Being the central part of the model, it is important to study the properties of coloured noise processes in more detail. Coloured noise is a Gaussian process and it is well known that these processes can be completely described by their mean and covariance functions see [14]. From Eq. (11) and from Fig. 1a, it is easily seen that the mean approaches zero throughout and therefore requires little attention. The covariance, however, depends not only on time but also on the initial values of $u_n(0)$ and $v_n(0)$. This immediately gives rise to the question of how to actually choose or determine these values. Let's consider the covariance matrix of the stationary process $\mathbf{u}$ in the stochastic differential equations of the form (13). It is known (see e.g.,[8]) that covariance function can now be described by

$$\frac{dP}{dt} = FP + PF^T + GQG^T. \tag{15}$$

By equating dP/dt to 0, we can find the steady state covariance matrix $\overline{P}$. This matrix can then be used to generate instances of coloured noise processes. This way of generating instances of u vector ensures that



(a) $\alpha 1 = \alpha 2 = \alpha 3 = \alpha 4 = 1$ (b) $\alpha 1 = \alpha 2 = \alpha 3 = \alpha 4 = 1$

(c) $\alpha 1 = \alpha 2 = \alpha 3 = \alpha 4 = 1$

Fig. 1. (a) The mean goes to zero and (b,c) the variance and auto-covariance of coloured noise processes started from non-stationary to stationary state.

the process is sampled at its stationary phase thus removing any artefacts due to a certain choice of start values that would otherwise be used. The auto-covariance is depicted in Fig. 1c. Note that the behaviour of a physical process in this case depends on the parameters in the Lagrangian auto-covariance. Of course short-term diffusion behaviour is controlled by the auto-covariance function. This provides room for the choice of parameters e.g., $\alpha_1, \alpha_2, \ldots$ The mean, variance and the auto-covariance are not stationary for a finite time t but as $t \to \infty$, they approach the limiting stationary distribution values as shown in Fig. 1a–c.

5. Modelling dispersion of pollution in shallow water by using coloured noise force

Let us consider the following stochastic differential equation,

$$\mathrm{d}X(t) \overset{\text{Itô}}{=} f(X(t),t)\mathrm{d}t + g(X(t),t)\mathrm{d}B(t). \tag{16}$$

As stated earlier, the model in Eq. (16) is not physically accurate. The shortcoming of these traditional particle models is caused by the fact that the driving noise in the stochastic differential equations (1)–(2) and (16) are modelled as Brownian processes and as a result, have independent increments for time periods $t \ll T_L$ (see e.g., [8,14,4]). Rather, for $t \ll T_L$ it is more realistic to assume that the increments are correlated. Therefore, for short time scales, a coloured force is applied so as to take into consideration the short time correlation behaviour.

5.1. The particle model forced by coloured noise

To model dispersion in shallow waters we have developed an extension of the particle model which is driven by coloured force. Such type of particle model is often referred to as the random flight model found in [1]. In this extension, the coloured noise process is generalised to $(u_n(t), v_n(t))$ which represents the velocity of the particle at time t in, respectively the x and y directions. This way the Lagrangian auto-covariance processes can be modelled more accurately by taking into account the characteristics of the turbulent fluid flow for $t \ll T_L$. By using the following set of equations the random flight model remains consistent with the advection–diffusion equation (6) for long period simulations while modelling accurately the short-term correlation of the turbulent fluid flows. In this application, unlike in [15], we choose longer length of the coloured noise, that is $n = 4$ and more experiments for simulations of the advection and diffusion of pollutants in shallow waters are carried out. Thus we use the following coloured noise:

$$\begin{aligned}
\mathrm{d}u_1(t) &= -\tfrac{1}{T_L}u_1(t)\mathrm{d}t + \alpha_1\mathrm{d}B(t), & \mathrm{d}v_1(t) &= -\tfrac{1}{T_L}v_1(t)\mathrm{d}t + \alpha_1\mathrm{d}B(t),\\
\mathrm{d}u_2(t) &= -\tfrac{1}{T_L}u_2(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_2 u_1(t)\mathrm{d}t, & \mathrm{d}v_2(t) &= -\tfrac{1}{T_L}v_2(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_2 v_1(t)\mathrm{d}t,\\
\mathrm{d}u_3(t) &= -\tfrac{1}{T_L}u_3(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_3 u_2(t)\mathrm{d}t, & \mathrm{d}v_3(t) &= -\tfrac{1}{T_L}v_3(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_3 v_2(t)\mathrm{d}t,\\
\mathrm{d}u_4(t) &= -\tfrac{1}{T_L}u_4(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_4 u_3(t)\mathrm{d}t, & \mathrm{d}v_4(t) &= -\tfrac{1}{T_L}v_4(t)\mathrm{d}t + \tfrac{1}{T_L}\alpha_4 v_3(t)\mathrm{d}t.
\end{aligned} \tag{17}$$

$$\begin{aligned}
\mathrm{d}X(t) &= \left[U + \sigma u_4(t) + \left(\frac{\partial H}{\partial x}D\right)\Big/H + \frac{\partial D}{\partial x}\right]\mathrm{d}t,\\
\mathrm{d}Y(t) &= \left[V + \sigma v_4(t) + \left(\frac{\partial H}{\partial y}D\right)\Big/H + \frac{\partial D}{\partial y}\right]\mathrm{d}t.
\end{aligned} \tag{18}$$

These systems of vector equations are Markovian we shall refer to this set of equations as the random flight model. The random flight model (17) and (18) is integrated for many different particles. Note that at the start of the simulation all particles have initial Gaussian velocities $(u_4(0), v_4(0))$ with zero mean and variance that agrees with covariance matrix $\overline{P}$ at a steady state.

6. The spreading behaviour of a cloud of contaminants

The characteristics of a spreading cloud of contaminants due to Brownian motion and coloured noise processes are discussed in the following sections.

6.1. Long-term spreading behaviour of clouds of particles due Brownian motion force

Let us, for now assume there is no drift term in Eq. (16) that is, $f(X(t),t) = 0$, and let

$$g(X(t),t) = \sqrt{2D}.$$

It follows that,

$$\mathrm{d}X(t) \overset{\text{Itô}}{=} \sqrt{2D}\mathrm{d}B(t). \tag{19}$$

By applying following theorem which is found in [11], that for any continuous function we have the following theorem.

Theorem 1. *Let $g(x)$ be continuous function and $\{B(t), t \geqslant 0\}$ be the standard Brownian motion process [11]. For each $t > 0$, there exits a random variable*

$$\mathscr{F}(g) = \int_0^t g(x)\mathrm{d}B(x),$$

which is the limiting of approximating sums

$$\mathscr{F}_n(g) = \sum_{k=1}^{2^n} g\left(\frac{k}{2^n}t\right)\left[B\left(\frac{k}{2^n}t\right) - B\left(\frac{k-1}{2^n}t\right)\right],$$

as $n \to \infty$. The random variable $\mathscr{F}(g)$ is normally distributed with mean zero and variance

$$\mathrm{Var}[\mathscr{F}(g)] = \int_0^t g^2(u)\mathrm{d}u,$$

if $f(x)$ is another continuous function of x then $\mathscr{F}(f)$ and $\mathscr{F}(g)$ have a joint normal distribution with covariance

$$\mathbb{E}[\mathscr{F}(f)\mathscr{F}(g)] = \int_0^t f(x)g(x)\mathrm{d}x.$$

to Eq. (19), it can be shown that the variance of a cloud of contaminants grows linearly with time:

$$\mathrm{Var}[X(t)] \overset{\text{Itô}}{=} 2Dt + \text{constant}. \tag{20}$$

For more detailed information as well as the proof of this theorem, the reader is referred to [11] for example.

6.2. Long-term spreading behaviour of clouds of contaminants subject to coloured noise forcing

As discussed in Section 5 with, for example, $u_1(t)$ from Eq. (11) as the coloured noise forcing and still assuming there is no background flow, the position of a particle at time t is given by

$$\mathrm{d}X(t) = \sigma u_1(t)\mathrm{d}t \quad \Rightarrow X(t) = X(0) + \sigma\int_0^t u_1(m)\mathrm{d}m. \tag{21}$$

For simplicity, yet without loss of generality, let $X(0) = u_i(0) = 0$, for $i = 1,2,\ldots,n$. Now, Eq. (11) leads to $u_1(m) = \alpha_1\int_0^m \mathrm{e}^{-\frac{1}{T_\mathrm{L}}(m-k)}\mathrm{d}B(k)$, and consequently,

$$X(t) \overset{\text{Itô}}{=} \sigma\alpha_1 T_\mathrm{L}\int_0^t \left(1 - \mathrm{e}^{-\frac{1}{T_\mathrm{L}}(t-k)}\right)\mathrm{d}B(k). \tag{22}$$

Using Theorem 1, the position of a particle at time t is normally distributed with zero mean and variance

$$\frac{\mathrm{Var}[X(t)]}{t} = \sigma^2\alpha_1^2 T_\mathrm{L}^2\left[1 - \frac{2T_\mathrm{L}}{t}\left(1 - \mathrm{e}^{\frac{-t}{T_\mathrm{L}}}\right) + \frac{T_\mathrm{L}}{2t}\left(1 - \mathrm{e}^{\frac{-2t}{T_\mathrm{L}}}\right)\right].$$

Thus, a position of a particle observed over a long time span as modelled by the coloured noise process $u_1(t)$ behaves much like the one driven by Brownian motion with variance parameter $\sigma^2\alpha_1^2T_\mathrm{L}^2$. Hence, the dispersion

coefficient is related to variance parameters $\sigma^2\alpha_1^2T_L^2 = 2D$. We can clarify this by considering Eq. (22), where the second part is $u_1(t)$ itself;

$$X(t) = \sigma T_L[\alpha_1 B(t) - u_1(t)], \quad \text{where } u_1(t) = \alpha_1 \int_0^t e^{-\frac{1}{T_L}(t-k)} dB(k).$$

Let us now rescale the position process in order to better observe the changes over large time spans. Doing so, for $N > 0$, we get

$$X_N(t) = \frac{1}{\sqrt{N}} X(Nt) = \sigma T_L \left[\alpha_1 \tilde{B}(t) + \frac{1}{\sqrt{N}} u_1(t)\right], \tag{23}$$

where $\widetilde{B}(t) = \frac{B(Nt)}{\sqrt{N}}$ remains a standard Brownian motion process. For sufficiently large N it becomes clear that Eq. (23) behaves like Brownian motion:

$$X_N(t) \approx \sigma\alpha_1 T_L \widetilde{B}(t).$$

6.3. The analysis of short-term spreading behaviour of a cloud of contaminants

For scalar coloured noise, it can be shown using Eq. (12) that

$$\mathrm{Cov}[u_{t+\tau}u_t] = \mathbb{E}[u_{t+\tau}u_t] = \mathbb{E}[v_{t+\tau}v_t] = \frac{1}{2}\alpha_1^2 T_L e^{\frac{-|\tau|}{T_L}}. \tag{24}$$

From Eq. (24), It follows that,

$$\mathbb{E}[u_\tau u_s] = \frac{1}{2}\alpha_1^2 T_L e^{\frac{-|\tau-s|}{T_L}},$$

$$\mathrm{Var}[X_t] = \sigma^2 \int_0^t \int_0^t \frac{1}{2}\alpha_1^2 T_L e^{\frac{-(\tau-s)}{T_L}} d\tau\, ds. \tag{25}$$

The integration of Eq. (25) can easily be yielded by separately considering the regions $\tau < s$ and $\tau > s$, and it can be shown that

$$\mathrm{Var}[X_t] = \sigma^2\alpha_1^2 T_L^3 \left(\frac{t^2}{2T_L^2} - \frac{t^3}{6T_L^3} \cdots\right) = \frac{\sigma^2\alpha_1^2 T_L t^2}{2} - \frac{\sigma^2\alpha_1^2 t^3}{6} + \cdots \tag{26}$$

Since we are interested only in the short time analysis, Eq. (26) is considered only for very small values of t in a sense that for $t \ll T_L$ the variance of a cloud of particles shortly after deployment is then given by the following equation:

$$\mathrm{Var}[X_t] = \frac{1}{2}\sigma^2\alpha_1^2 T_L t^2. \tag{27}$$

With the constant dispersion coefficient $D = \frac{1}{2}\sigma^2\alpha_1^2 T_L^2$, the variance of the cloud of particles, therefore initially grows with the square of time:

$$\mathrm{Var}[X(t)] = \frac{D}{T_L} t^2. \tag{28}$$

6.4. The general long-term behaviour of a cloud of contaminants due to coloured noise

Let us assume that there is no flow in the model and therefore have

$$dX(t) = \sigma u_1(t)dt \to X(t) = \int_0^t \sigma u_1(s) ds, \; u_1(s) = \alpha_1 \int_0^s e^{-\frac{1}{T_L}(s-k)} dB(k),$$

$$X(t) = \left(\frac{1}{T_L}\right)^0 \sigma\alpha_1 \int_0^t \int_0^{t-k} e^{-\frac{1}{T_L}(s-k)} \frac{(s-k)^0}{0!} ds\, dB(k), \quad X(0) = 0.$$

It can then be shown that

$$u_2(s) = \frac{1}{T_L}\alpha_1\alpha_2 \int_0^s e^{-\frac{1}{T_L}(s-k)}(s-k)\, dB(k), \tag{29}$$

where $0 < m < s < t$. Since $k < s$, the position of a particle due to coloured noise force Eq. (29) is given by

$$X(t) = \left(\frac{1}{T_L}\right)^1 \sigma\alpha_1\alpha_2 \int_0^t \int_0^{t-k} e^{-\frac{1}{T_L}(s-k)} \frac{(s-k)^1}{1!} ds\, dB(k).$$

In general, a position due to $u_n(t)$ force is $X(t) = \int_0^t \sigma u_n(s)\, ds$, and it follows that

$$X(t) \overset{\text{Itô}}{=} \left(\frac{1}{T_L}\right)^{n-1} \sigma \prod_{i=1}^n \alpha_i \int_0^t \left[\int_0^{t-k} e^{-\frac{1}{T_L}(s-k)} \frac{(s-k)^{n-1}}{(n-1)!}\right] ds\, dB(k). \tag{30}$$

Careful manipulation using integration by parts of the integral within the square brackets of Eq. (30), yields

$$X(t) \overset{\text{Itô}}{=} (T_L)^n \left(\frac{1}{T_L}\right)^{n-1} \sigma \prod_{i=1}^n \alpha_i \int_0^t [1 + \cdots] dB(k) \quad \text{for } n \geqslant 1. \tag{31}$$

Finally, with the aid of Theorem 1 whose proof is found in [11], the variance of a cloud of contaminants can be computed as described in the sections above. The derivation of velocity $v_n(t)$ of the particle along the y direction proceeds completely analogously. Let us now compute the variance of the general equations for position given by Eq. (31)

$$\mathrm{Var}[X(t)] = \sigma^2 (T_L)^2 \prod_{i=1}^n \alpha_i^2 \int_0^t [1 - \cdots]^2 dk. \tag{32}$$

For $\sigma > 0, \alpha_i > 0$, and $T_L > 0$, the process again behaves like a Brownian process with variance parameters $T_L^2\sigma^2\prod_{i=1}^n \alpha_i^2$ as $t \to \infty$. Thus the appropriate diffusion coefficient from Eq. (20) is equals $D = \frac{\sigma^2 T_L^2 \prod_{i=1}^n \alpha_i^2}{2}$. This relation is important because it gives a criterion for various choices of parameters α_i, $i = 1, \ldots, n$, $T_L > 0$. In a simulation the constant dispersion coefficient D often is specified whereas σ must be solved in terms of the other parameters.

7. Discrete version of the particle model driven by brownian motion

Analytical solutions of stochastic differential equations do not always exist due to their complexity and nonlinearity. Therefore, stochastic numerical integration schemes are often applied [13,2]. An example of a numerical scheme is the Euler scheme which, although not optimal in terms of order of convergence, is easy to implement and requires only $O(\Delta t)$ in the weak sense [9]. Here the time interval $[t_0, T]$ is discretised as $t_0 = 0 < t_1 < t_2 < \cdots < t_{n-1} < t_n = T$, with $\Delta(t_k) = t_{k+1} - t_k$, $\Delta B(t_k) = B(t_{k+1}) - B(t_k)$, for $k = 0, 1, \ldots, n$.

$$\overline{X}(t_{k+1}) = \overline{X}(t_k) + \left[U + \left(\frac{\partial H}{\partial x} D\right) \Big/ H + \frac{\partial D}{\partial x}\right] \Delta(t_k) + \sqrt{2D}\Delta B(t_k), \tag{33}$$

$$\overline{Y}(t_{k+1}) = \overline{Y}(t_k) + \left[V + \left(\frac{\partial H}{\partial y} D\right) \Big/ H + \frac{\partial D}{\partial y}\right] \Delta(t_k) + \sqrt{2D}\Delta B(t_k), \tag{34}$$

where $\overline{X}(t_{k+1})$ and $\overline{Y}(t_{k+1})$ are the numerical approximations of the $X(t_{k+1})$ and $Y(t_{k+1})$ positions respectively due to the traditional particle model. The noise increments $\Delta B(t_k)$ are independent and normally distributed $N(0, \Delta(t_k))$ random variables which can be generated using e.g., pseudo-random number generators. The domain information consisting of flow velocities and depth is computed using a hydrodynamic model known as Waqua see [10]. The flow averaged fields are only available on grid points of a rectangularly discretised grid and therefore, interpolation methods are usually used to approximate the values at other positions.

7.1. Boundaries

Numerical schemes such as the Euler scheme often show very poor convergence behaviour [9]. This implies that, in order to get accurate results, small time steps are needed thus requiring much computation. Another problem with the Euler (or any other numerical scheme) is its undesirable behaviour in the vicinity of boundaries; a time step that is too large may result in particles unintentionally crossing boundaries. To tackle this problem we define two types of boundaries. Closed boundaries representing boundaries intrinsic to the domain, and open boundaries which arise from the modeller's decision to artificially limit the domain at that location. Besides these boundary types we also define what happens if, during integration, a particle crosses one of these two borders;

- In case an open boundary is crossed by a particle, the particle remains in the sea but is now outside the scope of the model and is therefore removed;
- In case a closed boundary is crossed by a particle during the advective step of integration, the step taken is cancelled and the time step halved until the boundary is no longer crossed. However, because of the halving, say n times, the integration time is reduced to $2^{-n}\Delta t$, leaving a remaining $(1-2^{-n})\Delta t$ integration time. This means at least another $2^n - 1$ steps need to be taken at the new integration step in order to complete the full time-step Δt. This way, shear along the coastline is modelled;
- If a closed boundary is crossed during the diffusive part of integration, the step size halving procedure described above is maintained with the modification that in addition to the position, the white noise process is also restored to its state prior to the abandoned integration step. Again the process of halving the time step and continuing integration is repeated until no boundaries are crossed and the full Δt time step has been integrated.

8. Numerical experiments

Before applying both the traditional model (1)–(2) and the part model forced by coloured noise (17)–(18) to a real life pollution problem, we have created a domain for test problem. In this case, we have considered a channel domain with flow field (see Fig. 2). In order to compare the spreading behaviour of a cloud of contaminants some experiments using both particle models have been carried out. The Table 1 below summarises the simulation parameters that have been used in the experiments:

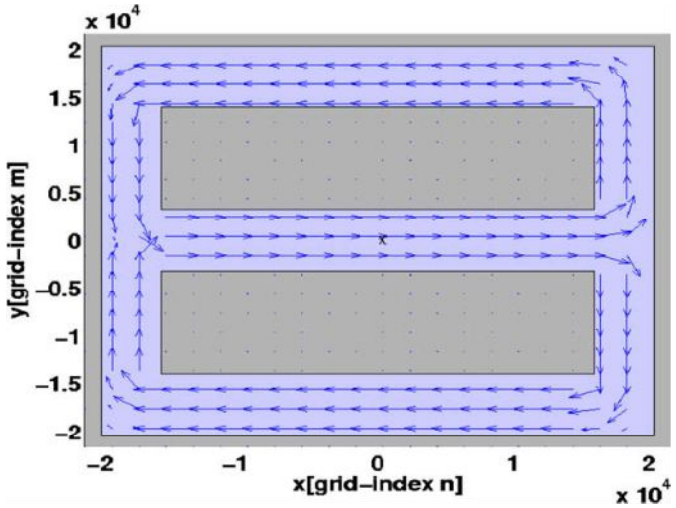


Fig. 2. Domain showing flow velocity and a point at which particles are released.

Table 1
The simulation parameters of the particle model for the dispersion of pollutants in shallow waters

Channel	Unit	Value	North sea	Unit	Value
# of steps	–	8999	#of steps	–	2499
Δt	s	864	Δt	s	864
Particles	–	40,000	Particles	–	400,000
α_1, α_2	–	$\alpha_1 = 1, \alpha_2 = 0.2$	α_1, α_2	–	$\alpha_1 = 1, \alpha_2 = 0.2$
α_3, α_4	–	$\alpha_3 = 1.2, \alpha_4 = 2$	α_3, α_4	–	$\alpha_3 = 1.2, \alpha_4 = 2$
Tracks	–	5	Tracks	–	5
Grid offset	m	(−21,600, −21,600)	grid offset	m	(40,550, 500,000)
Grid size	–	105 × 105	Grid size	–	201 × 201
Cell size	m	400 × 400	Grid size	m	800 × 800
Init. point	m	(0, 0)	Init. point	m	$(1.35 \times 10^5, 5.7 \times 10^5)$
D	m/s^2	3	D	m/s^2	3
T_L	s	30,000	T_L	s	30,000

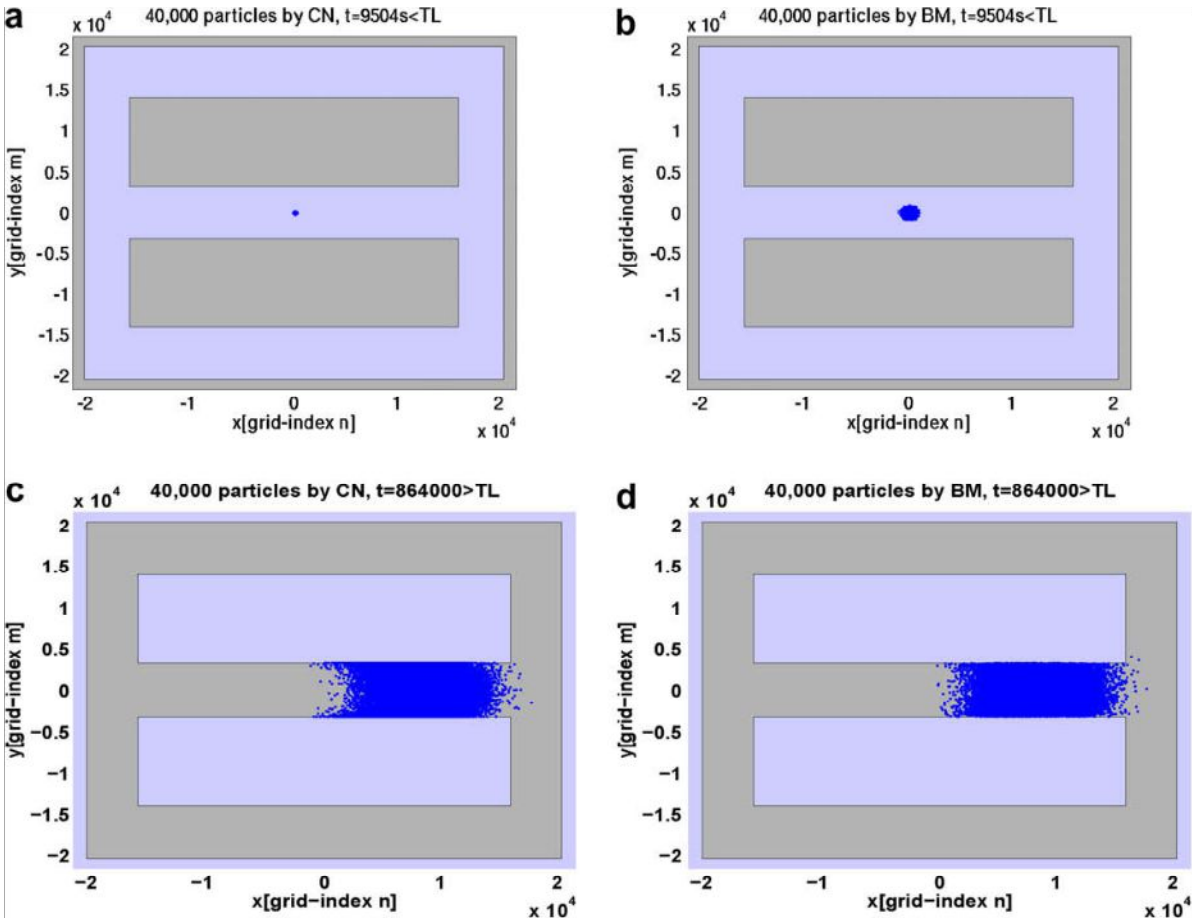


Fig. 3. Dispersion of a cloud of 40,000 particles released in the idealised channel domain. (a) Due to coloured noise for $t \ll T_L$, (b) due to Brownian motion noise for $t \ll T_L$, (c) due to coloured noise for $t \gg T_L$, and (d) due to Brownian motion noise for $t \gg T_L$.

9. Summary of the simulation parameters of particle for pollutants dispersion in shallow waters

From now onwards in this paper, we shall denote Brownian motion by BM and coloured noise by CN.

We release 20,000 particles at the center point (0, 0) marked by "X" and the simulation starts at time $t_0 = 0$ in the domain see Fig. 2. The scattering of a cloud of contaminants due to coloured noise or Brownian motions forces is followed at a specified time steps after release. Generally a large number of particles are used [4] in

numerical simulations. The simulations parameters that have been used for simulations of advection and diffusion of pollutants in shallow waters in this article are summarised in the Table 1. The channel domain Fig. 2 is

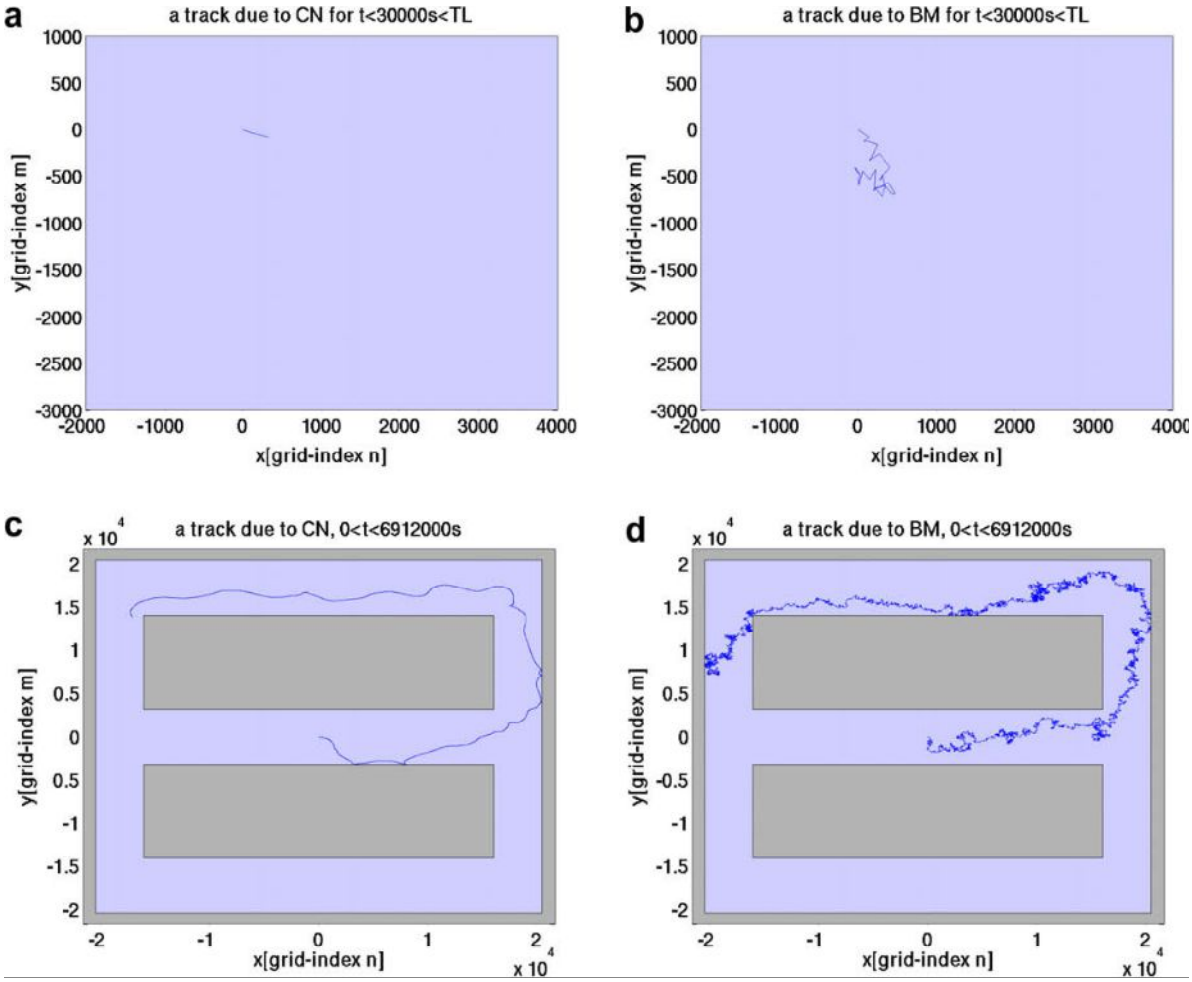


Fig. 4. Tracking of a single marked particle in the channel domain.

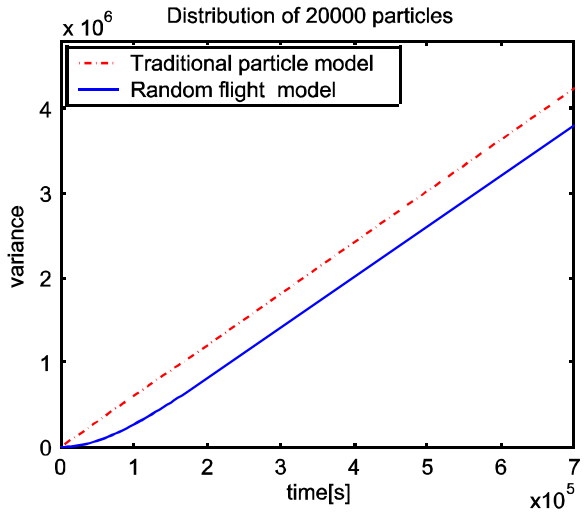


Fig. 5. The variance of a cloud of 20,000 particles in the idealised empty domain. There are two zones, one in which the variance grows quadratically with time for $t \ll T_L$ and another one it grows linearly with time for $t \gg T_L$.

mainly designed to discuss numerical problems that can be encountered in particle models see Section 7.1. The results in the Figs. 3a–d and 4a–d show that the spreading of a cloud of particles as well as a marked particle. By using the random flight model the short-term spreading is much smaller and moves persistently but slowly when you consider the temporal time scales $t : t \ll T_L$, while it is random and faster when you use Brownian motion.

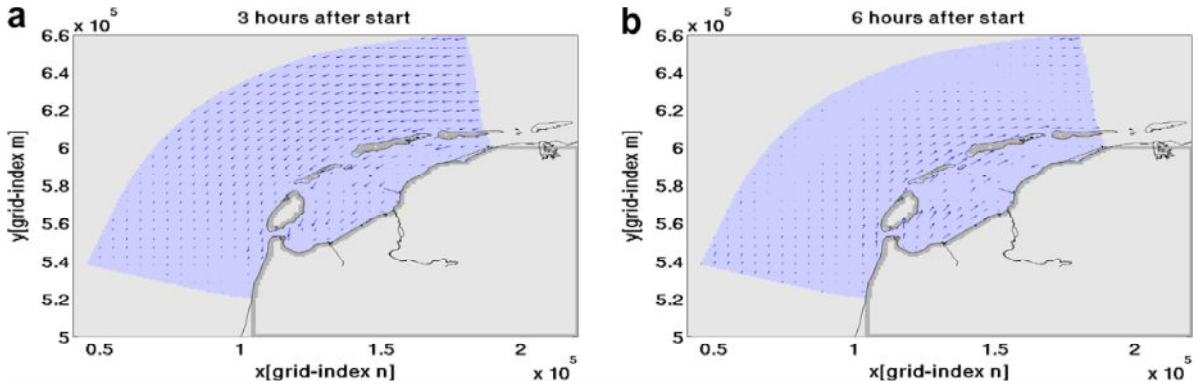


Fig. 6. (a) Example of tidally averaged flow fields 3 h after and (b) example of tidally averaged flow fields 6 h after.

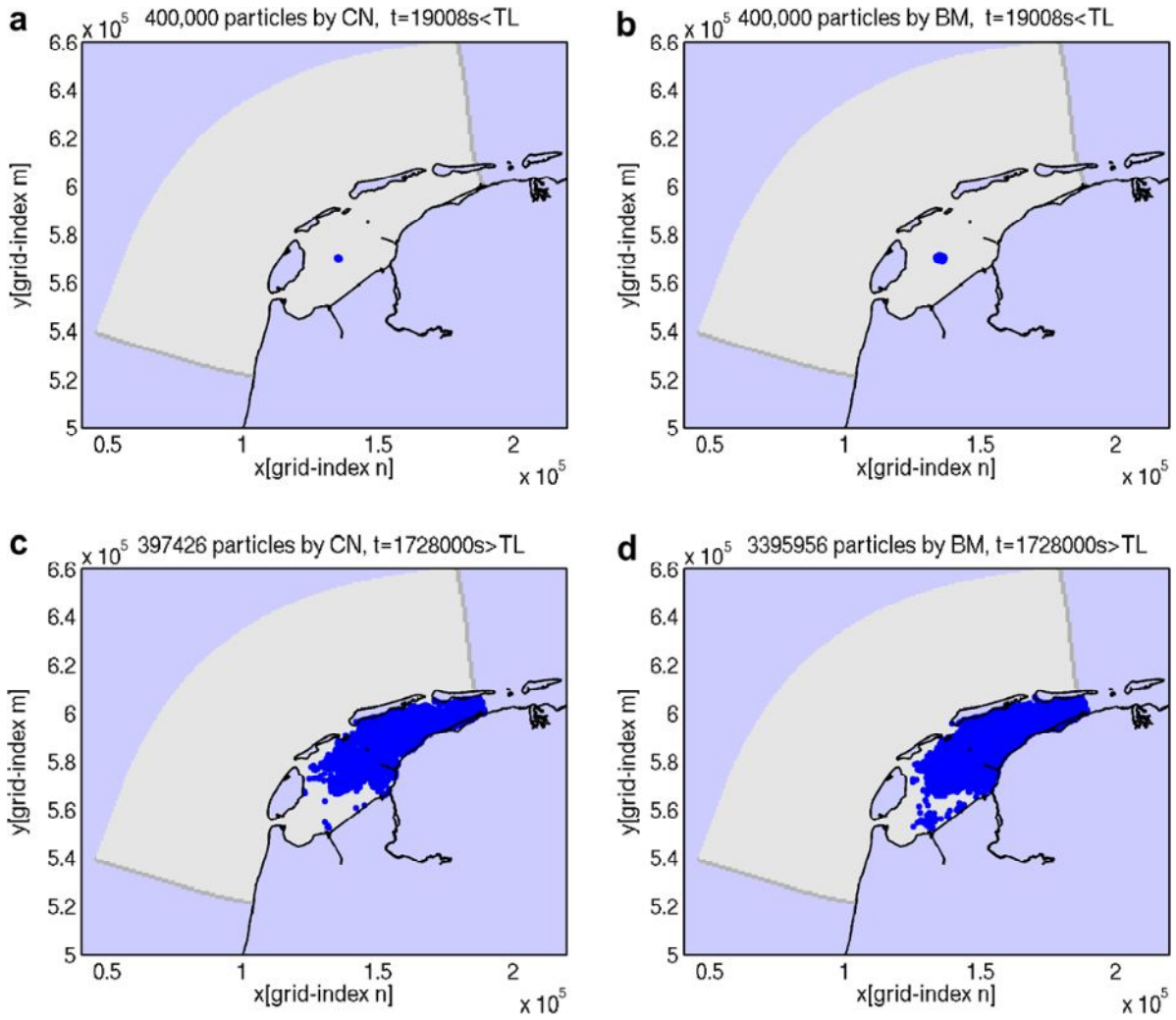


Fig. 7. (a, b) Dispersion of a cloud of 400,000 particles released at $(x, y) = (135\text{ km}, 570\text{ km})$ in the Wadden sea by the particle model due to coloured noise force for $t < T_L$ and (c, d) dispersion of a cloud of 400,000 particles released at $(x, y) = (135\text{ km}, 570\text{ km})$ in the Wadden sea the particle model driven by Brownian motion $t > T_L$.

However, in the long scale the spreading of a cloud has similar behaviours (see e.g., Fig. 3). This suggests that if one is interested in the accurate modelling in the short-term behaviour for $t : t \ll T_L$ then using the traditional particle model is not good, in that case it is better to use the random flight model [6].

In this paper, a series of experiments are carried out in a stationary homogeneous turbulent flow with zero mean velocity. The Lagrangian time scale as T_L is introduced in the models. We also did an experiment in the empty domain using random flight model as well as the traditional particle model so as to show the differences between the small scale fluctuations and their similarity in the long scale fluctuations. The simulation of the spreading of a cloud of 20,000 particles is tracked in an empty domain and its variance is computed. We have shown that once the particles have been in the flow longer than the time scale T_L, the variance of the spreading cloud grows linearly with time similar to the behaviour of the advection–diffusion equation. Before that time, the variance grows with the square of time (quadratically), creating two different zones of diffusion see Fig. 5. In Section 6.4 we have suggested that for $t \gg TL$ we can define a turbulent mixing coefficient similar to constant dispersion coefficient D such that $D = \frac{\sigma^2 T_L^2 \prod \alpha_i^2}{2}$.

10. Application of both particle model due to brownian and coloured noise respectively in the dutch coastal waters

For comparison purposes we have applied both models to the simulations of the dispersion of pollutants in the Dutch coastal waters in and around the Wadden sea. In this article, we choose a grid cell size of 800 m × 800 m this grid cell size is sufficiently small to model the dispersive effect of the tidal flow induced by topographic variations. The interpolation methods can be employed to get data at arbitrary positions, we have included few examples of the averaged flow field in the North sea (see Fig. 6). The spreading of a cloud of 400,000 particles is tracked see Fig. 7a–d, a cloud of contaminants is released from a fixed grid position and tracked by either a Brownian motion or a coloured noise force see Table 1, for the values of the simulation parameters.

11. Conclusions

The results show that the spreading of a cloud of particle for the short times scale is slow when it is driven by coloured noise force while it is much faster when it is driven by Brownian motion on the same scale. Therefore an improvement in modelling the dispersion of pollutants on a small time scale is achieved when a coloured noise force is employed. Thus, a particle model driven by coloured noise will provide the modeller with an enhanced tool for the short-term simulation of the pollutants by providing more flexibility to account for correlated physical processes of diffusion in the shallow waters. However, in this paper, a general analysis shows that a process observed over a long time spans as modelled by the coloured noise force behaves much like a Brownian motion model with variance parameter $\sigma^2 T_L^2 \prod_{i=1}^{n} \alpha_i^2$. The use of coloured noise, however, is more expensive in terms of computation and therefore it is advisable to use the particle model driven by coloured for short-term behaviour while adhering to the traditional particle model for long-term simulations.

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References

[1] A.W. Heemink, Stochastic modeling of dispersion in shallow waters, Stoch. Hydrol. Hydraul. 4 (1990) 161–174.
[2] J.W. Stijnen, A.W. Heemink, Numerical treatment of stochastic river quality models driven by colored noise, J. Water Resour. Res. 7 (39) (2003) 1–9.
[3] R.W. Barber, N.P. Volakos, Modelling depth-integrated pollution dispersion in the Gulf of Thermaikos using a Lagrangian particle technique, in: Proceedings of the 3rd International Conference on Water Resources Management, Portugal, WIT Trans. Ecol. Environ. 80 (2005) 173–184.

[4] P.S. Addison, Qu Bo, A. Nisbet, G. Pender, A non-Fickian particle-tracking diffusion model based on fractional Brownian motion, Int. J. Numer. Meth. Fluids 25 (1997) 1373–1384.
[5] D.J. Thomson, Criteria for the selection of stochastic models of particle trajectories in turbulent flows, J. Fluid Mech. 180 (1987) 529–556.
[6] H.B. Fischer, E.J. List, R.C.Y. Koh, J. Imberger, N.H. Brooks, Mixing in Inland and Coastal Waters, Academic Press, New York, 1979, pp. 1–483.
[7] J.R. Hunter, P.D. Crais, H.E. Phillips, On the use of random walk models with spatially variable diffusivity, J. Comput. Phys. 106 (1993) 366–376.
[8] A.H. Jazwinski, Stochastic Processes and Filtering Theory, Academic Press, New York, 1970, pp. 1–376.
[9] P.E. Kloeden, E. Platen, Numerical solutions of stochastic differential equations, Application of Mathematics, Springer-Verlag, New York, 2003, pp. 1–292.
[10] G.S. Stelling, Communications on Construction of Computational Methods for Shallow Water Flow Problems, Delft University of Technology, The Netherlands, Ph.D. Thesis, 1983.
[11] H.M. Taylor, S. Karlin, An Introduction to Stochastic Modelling, Academic Press, San Diego and California USA, 1998.
[12] C.W. Gardiner, Handbook of stochastic methods for physics, Chemistry and the Natural Sciences, Springer-Verlag, Berlin, 2004, pp. 1–409.
[13] G.N. Milstein, Numerical Integration of Stochastic Differential Equations, Kluwer Academic Publishers, 1995.
[14] L. Arnold, Stochastic differential equations, Theory and Applications, Wiley, London, 1974, pp. 1–228.
[15] W.M. Charles, A.W. Heemink, E. van den Berg, Stochastic particle models for transport problems in coastal waters, in: Proceedings of the 29th International Conference on Coastal Engineering, Lisbon, Portugal, WIT Transactions on The Built Environment, 1746-4498 78 (2005) 69–79.