Stochastic particle models for transport problems in coastal waters

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Abstract

In this paper transport processes in coastal waters are described by stochastic differential equations (SDEs). These SDEs are also called particle models (PMs). By interpreting a Fokker-Planck equation associated with the SDE as an advection diffusion equation (ADE), it is possible to derive the underlying PM which is exactly consistent with the ADE. Both the ADE and the related classical PM do not take into account accurately the short term spreading behaviour of particles. In the PM this shortcoming is due to the driving noise in the SDE which is modelled as a Brownian motion and therefore has independent increments. To improve the behaviour of the model shortly after the release of pollution we develop an improved PM forced by a coloured noise process representing the short-term correlated turbulent velocity of the particles. This way a more accurate and detailed short-term initial spreading behaviour of particles is achieved. For long-term simulations both the improved and classical PMs are consistent with the ADE. However, the improved PM is relatively easier to handle numerically than a corresponding ADE. In this paper both models are applied to a real life pollution problem in the Dutch coastal waters.
Keywords: Brownian motion, stochastic differential equations, particle models, coloured noise force, advection-diffusion equation, Fokker-Planck equation.

1 Introduction

Environmental management of shallow water areas requires a clear insight in the aftermath of, for instance, ship accidents or waste disposal. A good environmental control system must have the possibility to accurately predict the dispersion of pollutants. Particle models, play an important role in modelling transport phenomena



in shallow waters. The random forcing term of these models is usually a Brownian motion. Brownian motions processes are stationary Gaussian processes with independent increments with mean zero and variance Δt (Jazwinski [1]). These kinds of particle models are exactly consistent with an ADE (Heemink [2]). It is a well-known fact however that the ADE does only describe dispersion of particles in turbulent fluid flow accurately if the diffusing cloud of the particles has been in the flow longer than a certain Lagrangian time scale. This time scale (T_L) is the measure of how long it takes for a particle to lose memory of its initial turbulent velocity (Fischer *et al* [3]). In classical particle models turbulent fluid flow is simply modelled by Brownian motions as a result are unable to correctly describe the short term correlated behaviour found in real turbulent flows at sub-Lagrangian time scales. In this paper an extended correlated coloured noise process is employed as the driving force in the particle models. The inclusion of several parameters in the coloured noise process make it possible to adjust the auto-covariance to better match the physical processes. Furthermore, the improved particle model is developed in such a way that the coloured noise process approximates the Brownian motion over longer time periods. Therefore the improved particle model behaves the same as the classical particle model for long term simulations. This paper is organised as follows, in section 2 we briefly introduce the classical particle model. Section 3 introduces coloured noise processes. The improved particle model driven by coloured noise force is developed in section 4. The description of the modelling techniques of dispersion of pollution is given in section 4.1. The analysis of spreading properties such as variance of a cloud of particles are done from section 5. Finally, in section 6, both the classical and improved particle models are applied to a realistic prediction of the dispersion of pollution in the Dutch coastal waters.

2 The classical particle model for dispersion in shallow waters

Particle models describe the movement of a particle due to drift and diffusion terms. The position of a particle is denoted by $(X(t), Y(t))$ released in the water at time $t = 0$ at $(X(0), Y(0))$ for x respectively y direction at time t, and is given by

$$dX(t) \overset{\text{Itô}}{=} \left[U + \frac{D}{H}\frac{\partial H}{\partial x} + \frac{\partial D}{\partial x}\right] dt + \sqrt{2D}dB_1(t) \tag{1}$$

$$dY(t) \overset{\text{Itô}}{=} \left[V + \frac{D}{H}\frac{\partial H}{\partial x} + \frac{\partial D}{\partial y}\right] dt + \sqrt{2D}dB_2(t). \tag{2}$$

Where D is the dispersion coefficient in m^2/s, $U(x, y, t)$, $V(x, y, t)$ are the flow velocities along x, y direction respectively given in m/s, $H(x, y, t)$ is the total depth in m at a location (x, y), $dB(t)$ is a Brownian motion with mean $(0, 0)^T$ and $\mathbb{E}[dB(t)dB(t)^{\mathrm{T}}] = Idt$ where I is a 2×2 identity matrix (see Arnold [4]). At closed boundaries particle deflection occurs so that there is no loss of mass through such a boundary. The position $(X(t), Y(t))$ is Markov and the evolution

of its probability density function($p(x, y, t)$), is described by the Fokker Planck equation:

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

The initial location is very small we model it by using a Dirac delta function:

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

A particle concentration $C(x, y, t)$ is related to this $p(x, y, t)$:

$$C(x, y, t) = p(x, y, t)/H(x, y, t) \quad (5)$$

By substituting this into Fokker-Planck eqn. (3), the ADEs can be derived to be

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

An initial condition for the concentration can subsequently be obtained by substituting eqn. (4) into eqn. (5). By interpreting the Fokker-Planck equation eqn. (3) as an ADE makes the particle model in eqns. (1)- (2) consistent with advection-diffusion eqn. (6), (Heemink [2]).

3 Coloured noise processes

In this paper, the stochastic velocities of the particle induced by turbulent flow are called coloured noise forces.

3.1 The scalar exponential coloured noise process

Let a linear SDE for the dynamics of a velocity $u_1(t)$ of the particle be:

$$du_1(t) = -\frac{1}{T_L}u_1(t)dt + \alpha_1 dB(t). \quad (7)$$

$$u_1(t) = u_0 e^{\frac{-t}{T_L}} + \alpha_1 \int_0^t e^{-\frac{(t-s)}{T_L}} dB(s) \quad (8)$$

where $\alpha_1 > 0$ is constant and $u_1(t)$ is assumed to be stationary stochastic velocity induced by the turbulent fluid flow. For $t > s$ it can be shown (Jazwinski [1]), eqn.(8), has variance and Lagrangian auto-covariance of respectively,

$$\mathrm{Var}[u_1(t)] = \frac{\alpha_1^2 T_L}{2}(1 - e^{-\frac{2t}{T_L}}), \;\; \mathrm{Cov}[u_1(t), u_1(s)] = \frac{\alpha_1^2 T_L}{2}e^{-\frac{|t-s|}{T_L}}. \quad (9)$$

3.2 The general vector coloured noise force

The general linear SDEs for coloured noise processes are represented by

$$d\mathbf{u}(t) = \mathrm{F}\mathbf{u}(t)dt + \mathrm{G}(t)dB(t), \;\; d\mathbf{v}(t) = \mathrm{F}\mathbf{v}(t)dt + \mathrm{G}(t)dB(t). \tag{10}$$

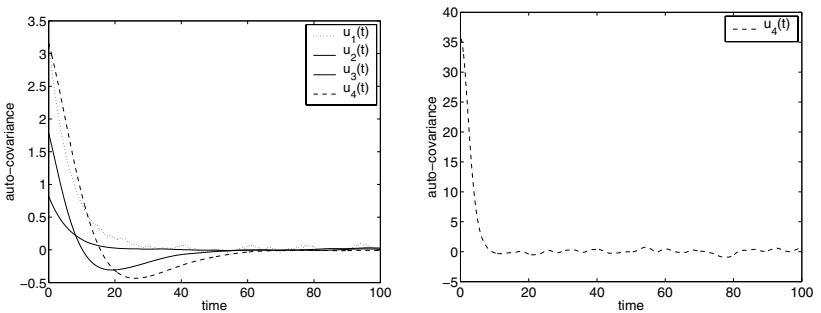
Here $\mathbf{u}(t)$ and $\mathbf{v}(t)$ are vectors of length n, F and G are n by n and n by m matrix functions respectively and $\{B(t); t \geq 0\}$ is an m-vector Brownian process. We express the coloured noise forcing along x direction:

$$du_1(t) = -\frac{1}{T_L}u_1(t)dt + \alpha_1 dB(t) \tag{11}$$

$$\cdots \qquad \cdots\cdots \qquad \cdots$$

$$du_n(t) = -\frac{1}{T_L}u_n(t)dt + \frac{1}{T_L}\alpha_n u_{n-1}(t)dt \tag{12}$$

Similar equations for $v_i(t), i = 1, \cdots, n$ along y direction can be found. The linear system in eqn.(10), is the same in the Itô and the Stratonovich sense. We integrate the coloured noise processes by the Heun scheme see e.g., (Kloeden and Platen [5]). Because the behaviour of a physical process depends on the parameters in



(a) $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1$ **(b)** $\alpha_1 = \alpha_2 = 1, \alpha_3 = 3, \alpha_4 = 5$

Figure 1: The auto-cavariance of coloured noise processes.

the Lagrangian auto-covariance in this model we provide a room for the choice of parameters e.g., $\alpha_1, \alpha_2 \cdots$ so as to alter their auto-covariance nature see fig. 1.

4 Improved particle model forced by coloured noise process

We use the coloured noise processes $u_2(t), v_2(t)$ as a forcing term:

$$\begin{aligned} du_1(t) &= -\tfrac{1}{T_L}u_1(t)dt + \alpha_1 dB(t) \\ du_2(t) &= -\tfrac{1}{T_L}u_2(t)dt + \tfrac{1}{T_L}\alpha_2 u_1(t)dt \\ dX(t) &= \left[U + \sigma u_2(t) + (\tfrac{\partial H}{\partial x}D)/H + \tfrac{\partial D}{\partial x}\right]dt \\ dv_1(t) &= -\tfrac{1}{T_L}v_1(t)dt + \alpha_1 dB(t) \\ dv_2(t) &= -\tfrac{1}{T_L}v_2(t)dt + \tfrac{1}{T_L}\alpha_2 v_1(t)dt \\ dY(t) &= \left[V + \sigma v_2(t) + (\tfrac{\partial H}{\partial y}D)/H + \tfrac{\partial D}{\partial y}\right]dt \end{aligned} \tag{13}$$

This is a Markov process and we call it an improved particle model.

4.1 Modelling dispersion of pollution processes by coloured forcing noise

Let us consider the following SDE,

$$dX(t) \overset{\text{Itô}}{=} f(X(t),t)dt + g(X(t),t)dB(t). \tag{14}$$

As stated earlier, the model in eqn. (14) is not physically accurate (Jazwinski [1]). To improve the model we use a coloured noise process $\{u_1(t)\}$ eqn (8) correlated with time to force the system:

$$\frac{dX(t)}{dt} = f(X(t),t) + g(X(t),t)u_1(t) \tag{15}$$

$$u_1(t) = -\frac{1}{T_L}u_1(t)dt + \alpha_1 dB(t) \tag{16}$$

The process $[X(t), u_1(t)]^{\mathrm{T}}$ is Markovian and can be interpreted in both the Itô or Stratonovich sense without affecting the outcome.

5 Analysis of long term behaviour of a cloud of particles

The statistical nature of the spreading cloud of particles due to Brownian motion and that due coloured noise processes is discussed in the following:

5.1 Long term of behaviour of Brownian motion force

Let us assume there is no drift term also $g(X(t),t) = \sqrt{2D}$ in eqn.(14):

$$dX(t) \overset{\text{Itô}}{=} \sqrt{2D}dB(t). \tag{17}$$

By applying thm.1 (see Appendix), on eqn. (17), we can show that the variance of a cloud of particle grows linearly with time:

$$\mathrm{Var}[X(t)] \overset{\text{Itô}}{=} 2Dt + \text{constant}. \tag{18}$$

5.2 Long term behaviour of a cloud of particles due to coloured noise forcing

We use the modelling techniques discussed in section 4.1 where we assume that $f(X(t),t) = 0$ and $g(X(t),t) = \sigma$ in eqn. (15), the position of a particle at time t:

$$dX(t) = \sigma u_1(t)dt, \quad \rightarrow X(t) = X(0) + \sigma \int_0^t u_1(m)dm. \tag{19}$$

For simplicity without loss of generality, let $X(0) = u_i(0) = 0$, for $i = 1, 2, \cdots, n$, eqn. (8), leads to $u_1(m) = \alpha_1 \int_0^m e^{-\frac{1}{T_L}(m-k)} dB(k)$, consequently.

$$X(t) \overset{\text{Itô}}{=} \sigma\alpha_1 T_L \int_0^t (1 - e^{-\frac{1}{T_L}(t-k)})dB(k). \tag{20}$$

Using thm.1,(see Appendix) the position of a particle at time t is normally distributed with zero mean and variance:

$$\frac{\text{Var}[X(t)]}{t} = \sigma^2\alpha_1^2 T_L^2 \left[1 - \frac{2T_L}{t}(1 - e^{\frac{-t}{T_L}}) + \frac{T_L}{2t}(1 - e^{\frac{-2t}{T_L}})\right]$$

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 that driven by Brownian motion with variance parameter $\sigma^2\alpha_1^2 T_L^2$. Hence, a dispersion coefficient is related with variance parameters: $\sigma^2\alpha_1^2 T_L^2 = 2D$. We elucidate this by considering eqn.(20), the second part is $u_1(t)$ itself:

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

Let us now rescale a position process so as to see changes better over large time spans. Accordingly, for $N > 0$, we get

$$X_N(t) = \frac{1}{\sqrt{N}} X(Nt) \; = \sigma T_L \left[\alpha_1 \tilde{B}(t) + \frac{1}{\sqrt{N}} u_1(t)\right], \tag{21}$$

where $\tilde{B}(t) = \frac{B(Nt)}{\sqrt{N}}$ remains a standard Brownian motion process. For $t \gg T_L$, $e^{-\frac{2t}{T_L}} < 1$ thus, the variance of $u_1(t) = \frac{\alpha_1^2 T_L}{2}(1 - e^{-\frac{2t}{T_L}}) \leq \frac{\alpha_1^2 T_L}{2}$, and the variance of $\frac{1}{\sqrt{N}} u_1(t)$ becomes negligible for large N. Eqn.(21), shows clearly how a process behaves like Brownian motion for large N,

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

5.3 Long term behaviour of a cloud of particles due to $u_2(t)$ forcing

We use the coloured noise forcing $u_2(t)$ and similar ways as in 5.2:

$$dX(t) = \sigma u_2(t)dt, \;\; u_2(s) = u_2(0)e^{-\frac{1}{T_L}s} + \frac{1}{T_L}\int_0^s \alpha_2 u_1(m)e^{-\frac{1}{T_L}(s-m)}dm. \tag{22}$$

$u_1(m) = \alpha_1 \int_0^m e^{-\frac{1}{T_L}(m-k)}dB(k)$. So, a velocity of the particle at time t is :

$$u_2(s) = \frac{1}{T_L}\alpha_1\alpha_2 \int_0^s e^{-\frac{1}{T_L}(s-k)}(s-k)dB(k), \tag{23}$$

where $0 < m < s < t$, and since $k < s$, therefore we can integrate from k to t:

$$X(t) = \frac{1}{T_L}\alpha_1\alpha_2\sigma \int_0^t \left[\int_k^t e^{-\frac{1}{T_L}(s-k)}(s-k)ds\right] dB(k), \;\; \text{thus}$$

$$X(t) \overset{\text{Itô}}{=} \alpha_1\alpha_2\sigma T_L \int_0^t \left[1 - e^{-\frac{1}{T_L}(t-k)} - \frac{1}{T_L}(t-k)e^{-\frac{1}{T_L}(t-k)}\right] dB(k). \tag{24}$$

By again applying theorem 1 (see Appendix), the variance becomes:

$$\text{Var}[X(t)] = \alpha_1^2\alpha_2^2\sigma^2 T_L^2 \int_0^t \left[(1 - e^{-\frac{1}{T_L}(t-k)}) - \frac{1}{T_L}(t-k)e^{-\frac{1}{T_L}(t-k)}\right]^2 dk.$$

Clearly from this equation we see that for $t \gg T_L$, i.e., $t \to \infty$, the particle's position due to $u_2(t)$ behaves like that of Brownian motion with variance parameter $\sigma^2\alpha_1^2\alpha_2^2T_L^2$.

5.4 General long term behaviour of a cloud of particles due to coloured noise

Let us assume that $f(X(t), t) = 0$ and $g(X(t), t) = \sigma$ in eqn. (15):

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

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

The position of a particle by a coloured noise force $u_2(t)$ eqn. (23), is :

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

In general, a position by a $u_n(t)$ force is: $X(t) = \int_0^t \sigma u_n(s)ds$, Therefore,

$$X(t) \overset{\text{Itô}}{=} \left(\frac{1}{T_L}\right)^{n-1} \sigma \prod_{i=1}^n \alpha_i \int_0^t [\int_0^{t-k} e^{-\frac{1}{T_L}(s-k)}\frac{(s-k)^{n-1}}{(n-1)!}]dsdB(k) \tag{25}$$

The derivations of velocity $v_i(t)$ of the particle along y direction proceed similarly. Upon manoeuvring integration by parts of the integral in the square brackets of

eqn. (25), we can get

$$X(t) \overset{\text{Itô}}{=} (T_L)^n \left(\frac{1}{T_L}\right)^{n-1} \sigma \prod_{i=1}^{n} \alpha_i \int_0^t [1....]\, dB(k), \quad \text{for } n \geq 1. \tag{26}$$

Finally with the aid of thm. 1, the variance of a cloud of particles can generally be computed as in the sections above. Let us compute the variance of the general equations for positions eqn. (26)

$$\text{Var}[X(t)] = \sigma^2 (T_L)^2 \prod_{i=1}^{n} \alpha_i^2 \int_0^t [(1 - .....]^2\, dk \tag{27}$$

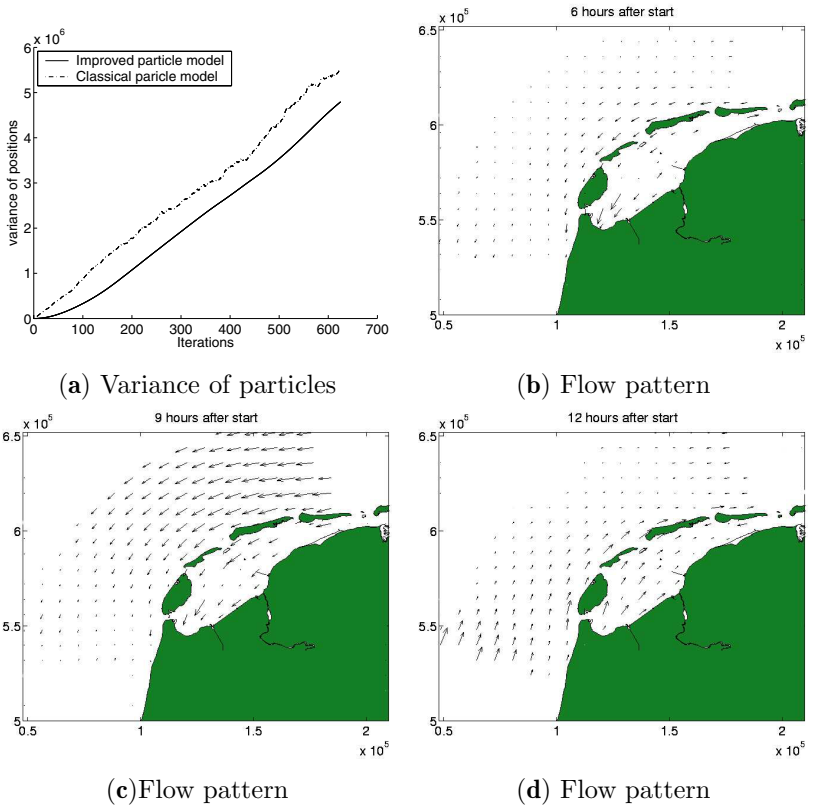
For $\sigma > 0,\ \alpha_i > 0,\ T_L > 0$, again as $t \to \infty$ the process behaves like a Brownian processes with $T_L^2 \sigma^2 \prod_{i=1}^{n} \alpha_i^2$. Thus the diffusion coefficient using eqn.(18), equals: $D = \frac{\sigma^2 T_L^2 \prod_{i=1}^{n} \alpha_i^2}{2}$.

6 Application of classical and the improved particle models to water pollution problem

For comparison purposes we have employed both models in the Dutch coastal waters mainly in the Wadden sea. We use real data computed by a hydrodynamical model known as Waqua see e.g., Stelling [6]. The bilinear interpolation method is employed to get data at arbitrary positions as we track the particle. The sample flow pattern see figures 2 (**b**)-(**d**). The variance of a cloud of 600 particles is computed to show the difference in the initial short term behaviours 2 (**a**). Figure 3 (**a**) contains a marked particle tracked by a coloured noise force $(u_2(t), v_2(t))$ initially released from grid position $(135000m, 570000m)$ at time t=0. Tracked by both models with parameters summarized in table 1. The subsequent tracking of the same marked particle after release shows that the particle tracked by coloured noise forcing tend to proceed in the current direction thus more persistent compared that by a Brownian motion. However for a large iteration value we see similar patterns, see figs. 3 (**c**) and 3(**d**)

Table 1: Summary of the parameters used in the program.

Sim. parameter	Grid data	Particle model
time = $0 - 7776000s$	cell size = $1000m \times 1000m$	$T_L = 34560s$
stepsize = $69.12s$	grid offset = $40550.0, 500000.0$	$\alpha_1 = \alpha_2 = 1$
iter. = 112499	grid size = 161×180	$\sigma = 0.0001$
particles = 5		$D = 5.971968m^2/s$
tracks = 5		



(**a**) Variance of particles (**b**) Flow pattern

(**c**)Flow pattern (**d**) Flow pattern

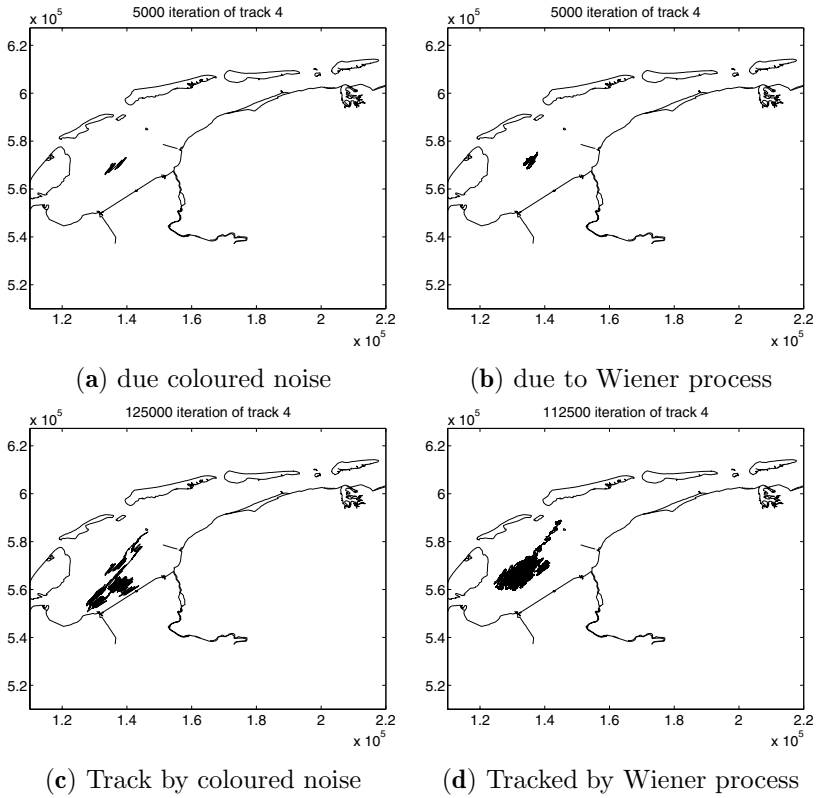
Figure 2: Sample of tidally flow fields in Dutch coastal.

7 Conclusions

The improved particle model which incorporates coloured noise process will provide the modeller with an enhanced tool for the short term simulation of the pollutant by providing more flexibility to account for correlated physical processes of diffusion in the environmental. 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 improved PM only for short term behaviour while adhering to the classical PM for long-term simulations.

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(**a**) due coloured noise (**b**) due to Wiener process

(**c**) Track by coloured noise (**d**) Tracked by Wiener process

Figure 3: Tracking of marked particles released in the Wadden sea.

Appendix

It is well known (Taylor and Karlin [7]), that for any continuous function we have the following theorem.

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

$$\mathcal{F}(g) = \int_0^t g(x)dB(x),$$

which is the limiting of approximating sums

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

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

$$\mathrm{Var}[\mathcal{F}(g)] = \int_0^t g^2(u)du.$$

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