A Lagrangian Model For Simulating The Dispersal Of Sand-Sized Particles In Coastal Waters

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Abstract

A model, SandTrack, has been established to simulate movements of sand-sized particles in coastal waters within a Lagrangian framework. The model can be applied to assess the dispersal of contaminated particulate material, such as may be associated with industrial discharges, or the dispersal of dredged spoil. For such applications, the Lagrangian approach is essential, as the identity of the particles is important. Although Lagrangian models existed previously which could simulate fine sediment constantly in suspension, there are certain applications, such as dealing with the movement of bed particles, in which intermittent physical processes are critical. SandTrack has been tested against field observations from the coastal waters near Dounreay, United Kingdom. The tests strengthened confidence in the model predictions, and enabled appropriate values of some of the model's main physical parameters to be set. Some features of the particle distributions simulated by SandTrack are consistent with field observations, and are not achievable with simpler sediment transport models. The model's run times are sufficiently short for simulations of particle movement in moderately large coastal areas over several decades to be practical.

Introduction

Conventional Eulerian transport models predict the bulk flux of sand-sized particles in the sea, ignoring the identity of the particles. However, for certain problems, a Lagrangian approach is required, as the identity of the particles is important. Such problems include studies of the dispersal of contaminated particulate material, such as may be associated with industrial discharges, and of the dispersal of dredged spoil. Existing Lagrangian models for very fine sediments, such as SEDPLUME-RW (Mead 1991; Mead and Rodger 1991) and SEDTRAIL-RW (Spearman et al 2006), whilst being suited to the purpose for which they were designed, do not include particle trapping in the seabed, bedload transport or incipient motion. A model, SandTrack, has been devised to simulate movements of sand-sized particles, or "tagged" particles, within a Lagrangian framework. We distinguish *tagged* particles (or grains), being the ones which are of interest and are tracked, from the *indigenous* grains, being the natural local sediments around the tagged grains. Each tagged grain could be representative of many thousands of similar grains.

SandTrack was developed originally between 2001 and 2005 to address concern which had arisen regarding the movement of bed sediment in the coastal waters around the Nuclear Facility at Dounreay on the north coast of Scotland. The primary concern was related to the dispersion of sand-sized particles, which may have originated from the vicinity of the Dounreay outfall diffuser. These particles, which arose from industrial processes associated with research undertaken at the Facility, have become integrated with the local sediments on the seabed. They have approximately the same size and shape as the local sediments, but the density of the particles is generally slightly higher; the particles have specific gravities in the range 2.6 to 3.0, compared with the specific gravity of the native sand of 2.65. The local sediments, mainly non-cohesive sands, are subject to re-suspension and transport dominated by a combination of waves and tidal currents. Thus, it is believed that the industrial particles will have behaved in a similar way to local sand particles, and will have been dispersed from their source following the pre-existing sediment transport pathways along this stretch of coastline. The tagged grains whose movement is modelled by SandTrack may have a different diameter, d_t, and density, $\rho_{s,t}$, to the indigenous sand grains comprising the seabed of diameter, d_a, and density, $\rho_{s,a}$.

The capabilities of SandTrack are broadly similar to those of the Particle Tracking Model (PTM) presented by MacDonald and Davies (2006), Lackey and MacDonald (2007) and Gailani et al (2007). However, SandTrack was developed completely independently of the PTM, and details of the model formulations differ. Some comparisons of PTM results with field data have been undertaken, but the data were insufficient to complete adequate comparisons for sand-sized sediment (Gailani et al 2007).

Applications of SandTrack have been presented by Soulsby et al (2006; 2007). On the basis of comparisons between SandTrack results and field data, including Dounreay industrial particle recoveries and tracer dispersal data from another United Kingdom site, the authors concluded that the model can reproduce the main features and speeds of sand-sized particle dispersal in coastal waters. In contrast to Soulsby et al (2006; 2007), the present paper focuses on the detailed mathematical formulation of SandTrack. Following a description of the model formulation, the paper covers model tests against field data and presents some predictive model runs, before drawing conclusions. Some of the SandTrack algorithms are drawn from "Dynamics of Marine Sands" (Soulsby 1997), which is referred to hereafter as DMS.

Model formulation

The use of Lagrangian modelling techniques in marine applications has been discussed by numerous authors, including Hunter (1987) and Mead (1991, 2004). Lagrangian models represent substance releases to the sea as regular releases of discrete particles, each representing a defined quantity of the released substance. Model particles move under the influence of currents simulated by numerical hydrodynamic models.

For most marine applications, particles in Lagrangian models are advected at the speeds of prevailing currents. However, in SandTrack, each model particle is identified with a grain of released material, and the grain speed, U_{gr}, is used. This is taken to be given by the product of certain functions F, P and R, all related to grain mobility, which are formulated in terms of the wave, current and sediment characteristics later:

$$U_{gr} = F \cdot P \cdot R \cdot U_c \qquad (1)$$

Where U_{gr} is the mean speed of a mobile grain during a model timestep;
F is a "freedom factor", with F=0 if the grain is buried or trapped, and F=1 if the grain is at or near the surface of the bed, and hence free to move;
P is the probability (or, equivalently, proportion of time) that a free grain is moving as bedload or in suspension, with $0 \leq P \leq 1$;
R is a reduction factor for the speed of a mobile grain compared with U_c, with $0 \leq R \leq 1$; and
U_c is the current speed averaged over the lowest 1m of the water column.
In the two horizontal dimensions used by SandTrack, U_{gr} and U_c are vectors, with $\underset{\sim}{U}_{gr}$ aligned with $\underset{\sim}{U}_c$.

Equation (1) differs from conventional sediment transport formulae in that it represents the movement of individual grains, whereas sediment transport formulae predict the bulk movement of grains regardless of their identity. Nevertheless, Equation (1) has parallels with sediment transport formulae which are drawn on later.

Functions F, P and R, and the speed, U_c, all vary with the positions of individual grains (and so reflect the varying exposure of the grains to wave and current velocities) and with time. They are specified in terms of the Shields parameters embodying the mobility of the grains, $\theta_{max,a}$ and θ_{max} (the maximum Shields parameter during a wave cycle under combined waves and current, for the indigenous and tagged grains respectively), in comparison with threshold Shields parameters ($\theta_{cr,a}$ for the indigenous grains, and $\theta_{cr,A}$ for a tagged grain on a bed of indigenous grains). The functions also depend on a number of constant parameters which are either calculated for the indigenous and tagged grains, or are fixed, calibrated coefficients.

Specification of function F

Burial, or trapping, of tagged particles in the seabed, and subsequent release, are important processes in determining ultimate particle distributions. An early version of SandTrack (Soulsby et al 2007) modelled changes in seabed level, and hence depths of burial of tagged grains, using a vertical random walk. A mechanistic model to relate the movement of particles up and down in the bed to the main driving processes and the local nature of the bed via ripple, sandwave and suspension dynamics was explored, but this proved to be too dependent on a large number of poorly-understood parameters. The present SandTrack burial/trapping algorithm is, therefore, based on the concept that, as far as the particle-tracking model is concerned, a particle is simply either trapped (F=0) or free to move (F=1). A trapped particle might be buried in a sandy seabed, trapped in a rock fissure, trapped in a kelp bed, or subject to any other mechanism that prevents it from moving. However, it is also assumed that the process that caused the particle to become trapped can be reversed so that it becomes free; that is, able to move. During an interval of unit time (taken as one second), there is a transition probability "a" that a trapped particle becomes free, and a different transition probability "b" that a free particle becomes trapped. It follows that the probability that a trapped particle remains trapped (during the time interval) is (1-a), and that a free particle remains free is (1-b). If Δt is the model timestep in seconds, then the probabilities of transition during Δt are $a\Delta t$, $b\Delta t$, $(1-a)\Delta t$ and $(1-b)\Delta t$. This allows a "natural" timescale, related to a typical residence time in the seabed, to be introduced.

If the proportion of particles that are free is denoted by γ, then the long-term equilibrium value of γ (for fixed values of a and b) is:

$$\gamma_e = a/(a+b) \tag{2}$$

The probabilities a and b need to be related to the hydrodynamic parameters, such that: particles will only change from free to trapped (or trapped to free) when the indigenous sediment is mobile, that probabilities of transitions free-to-trapped (or trapped-to-free) increase with wave and current activity, and that probabilities are reduced (and hence residence times are longer) in deeper water. Since these transitions are not easily observable, the following functional dependencies of a and b were devised, so that their use results in the transition probabilities increasing with $\theta_{max,a}$; from b=0 at $\theta_{max,a}=\theta_{cr,a}$, to $b=b_e$ for $\theta_{max,a} >> \theta_s$:

$$b = 0 \qquad \text{if } \theta_{max,a} \le \theta_{cr,a} \tag{3}$$

$$ = b_e\left[1 - \exp\{-(\theta_{max,a} - \theta_{cr,a}) / \theta_s\}\right] \qquad \text{if } \theta_{max,a} > \theta_{cr,a} \tag{4}$$

$$a = \gamma_e.b / (1-\gamma_e) \tag{5}$$

a and b thus depend on three tuneable parameters: the long-term equilibrium proportion of particles which are free, γ_e; the maximum free-to-trapped transition probability, b_e; and the scale value, θ_s, which determines the distribution of residence times. The critical value of the Shields parameter, $\theta_{cr,a}$, must be exceeded (usually during storms) in order for transitions to be made. Equation (5), derived from Equation (2), ensures that the equilibrium proportion of free particles is γ_e. The calibration of values of the free parameters γ_e, θ_s and b_e using observations from Dounreay is described later. Note that a and b are related to the Shields parameter and threshold Shields parameter, $\theta_{max,a}$ and $\theta_{cr,a}$ respectively, for the *indigenous* sediment, since these determine by how much and how quickly the bed level changes.

Specification of function P

A particle in the surface layer of the seabed (that is, with F=1) will remain at rest at a particular location and time if the prevailing wave and current conditions are insufficient to move it. This is tested by comparing the maximum Shields parameter under combined waves and current, θ_{max}, for the tagged grains with the threshold value for the tagged grains, $\theta_{cr,A}$ (defined later). For shear stresses in excess of the threshold values, particles will be moved, with a larger proportion of the available particles being moved by a larger excess stress, until all the grains are in motion. The motion may be as bedload or by suspension. In terms of a single tagged grain, this is equivalent to specifying the probability that the tagged grain will move. During a model timestep, Δt, P can be regarded as the fraction of this time that the grain is moving.

The probability of motion function, P, is defined by adapting an expression, applicable to steady currents, given by Fredsøe and Deigaard (1992) (hereafter FD92), which is based on the methods of Engelund and Fredsøe (1976) (hereafter EF76). Madsen (1991) derived an expression for the response time of a grain to a sudden change in the flow and concluded that bedload transport responds virtually instantaneously compared to the timescale of coastal wave motions. We therefore adopt the steady-flow expression, and apply it in a quasi-steady fashion to wave-plus-current conditions, by replacing FD92's with θ_{max}, to represent the "mobility" factor of the tagged grains under combined waves and currents, yielding:

$$\begin{aligned} P &= \left[1+\left(\frac{\frac{\pi}{6}\mu_d}{\theta_{max}-\theta_{cr,A}}\right)^4\right]^{-1/4} &&, \text{if } \theta_{max} > \theta_{cr,A} \\ &= 0 &&, \text{if } \theta_{max} \le \theta_{cr,A} \end{aligned} \qquad (6)$$

The variation of P with θ_{max} is illustrated in Figure 1a for tagged grains of 0.25mm diameter. FD92 gave various values for the dynamic friction coefficient, μ_d, ranging between 0.5 and 1.0. For SandTrack, a value of $\mu_d = 0.5$ was selected, which gave the best match with conventional sediment transport methods.

Function R

A particle that is moving (F=1, P>0) travels with a speed that depends on the wave and current flow velocities. When the bed shear stress is just above the threshold value, the particle rolls or hops along the bed in bedload motion, at a speed of typically 15% of the current speed near the bed (FD92). Its speed increases with the bed shear stress up to a maximum of about 50% of the near-bed current speed. If its settling velocity is sufficiently small, it is carried into suspension by the vertical turbulent motions, and if it is carried high enough, it could move at a speed equal to that of the near-bed current. In SandTrack, it is assumed that all the particles travel within the bottom 1m of the flow, and accordingly the particle speed is related to the depth-averaged current speed in the bottom 1m (or the depth-averaged speed over the water depth, where this is less than 1m).

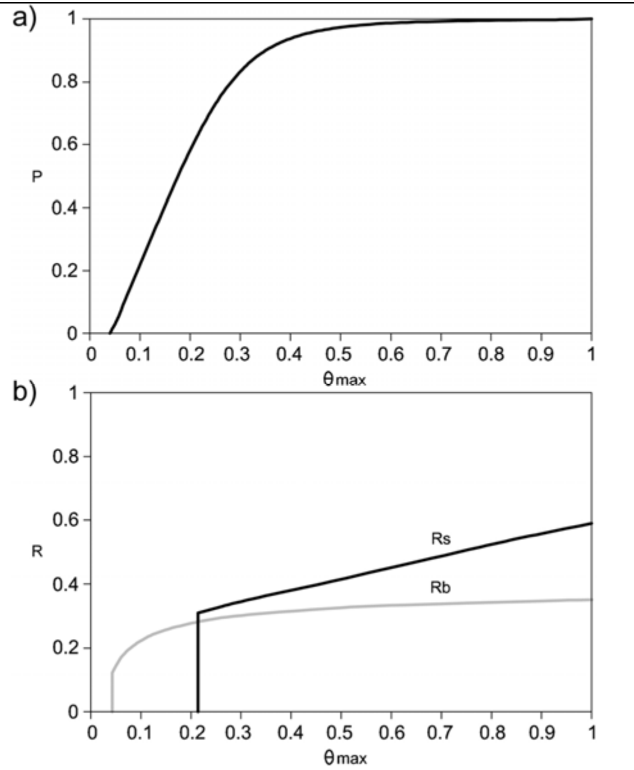

Figure 1. Variations with θ_{max} of the functions (a) P, and (b) R for 0.25mm grains

Bedload transport

The function, R, used by SandTrack is based on an equation given by FD92. Again, this is taken from the bedload transport method developed by EF76. As with Equation (6), we have used Madsen's (1991) conclusion in assuming that the steady-flow expression of FD92 and EF76 can be adapted to the wave-plus-current case by (a) replacing u_* with the mean friction velocity over a wave cycle, u_{*m}, outside the brackets, because this corresponds to a transporting term, and (b) replacing θ with θ_{max} inside the brackets, because here it is used as a mobilising term. Then the speed, U_b, of a particle undergoing bedload transport is given by:

$$U_b = 10u_{*m} \left[1 - 0.7(\theta_{cr,A}/\theta_{max})^{1/2} \right] \qquad (7)$$

Then function R for bedload transport, $R_b = U_b/U_c$, is given by:

$$\begin{aligned} R_b &= 10u_{*m}\left[1-0.7\left(\theta_{cr,A}/\theta_{max}\right)^{1/2}\right]/U_c && \text{, if } \theta_{max} > \theta_{cr,A} \\ &= 0 && \text{, if } \theta_{max} \le \theta_{cr,A} \end{aligned} \qquad (8)$$

Suspended transport

Particles can only be carried into suspension if the upward turbulent velocity motions of the water exceed the terminal settling velocity, w_s, of the particles. Vertical turbulent velocities are closely related to the maximum friction velocity, u_{*max}, and the criterion to determine whether particles can be suspended is taken as:

$$u_{*max} > w_s \qquad (9)$$

If one defines the Rouse parameter, $B=w_s/(0.4u_{*max})$, then Equation (9) indicates that particles are suspended if B<2.5. In this case, SandTrack assumes that all the particles travel in suspension (this assumption is discussed further below). They are thus able to travel at heights above the bed where the flow velocity is larger. If U(z) and C(z) denote variations of horizontal velocity and concentration of suspended particles respectively with height, z, above the seabed, then the weighted-mean horizontal velocity of suspended particles, U_s, is given by:

$$U_s = \frac{\int_{z_1}^{z_2} U(z)\,C(z)\,dz}{\int_{z_1}^{z_2} C(z)\,dz} \qquad (10)$$

where z_1 is taken as the thickness of the bedload layer, given as the height at which $U(z_1)=R_bU_c$, and z_2 is taken as 1m, which is the upper limit for suspended transport assumed in the present model (for finer sediments, when suspended transport may be more significant, the more traditional modelling approaches described previously can be used).

Substituting $U(z)\sim z^{1/7}$ and $C(z)\sim z^{-B}$ (following DMS) into Equation (10) gives, after some mathematics, an expression for R_s:

$$R_s = \frac{R_b(1-B)}{\left[(8/7)-B\right]} \cdot \frac{\left[(8/7R_b)^{(8-7B)} - 1\right]}{\left[(8/7R_b)^{(7-7B)} - 1\right]} \qquad (11)$$

where $R_s=U_s/U_c$, and R_b is given by Equation (8). Equation (11) shows that the speed of the average suspended particle is only slightly larger than the bedload speed, R_bU_c, for values of B approaching the threshold of suspension (B=2.5). Such B values correspond to large particles or low current and wave velocities. As the value of B becomes smaller (small particles, high flow speeds) the value of R_s increases to 1, and for very small B the particles travel at almost the same speed as the water in the lowest 1m layer. It is mathematically possible for R_s to slightly exceed 1 (because $z_1>0$); in such cases a limiting value of $R_s=1$ is applied.

The value of the relative speed function, R, is taken as R_b if $B\geq2.5$, or R_s if $B<2.5$. Figure 1b shows an example of the variation of R with θ_{max} for tagged grains of 0.25mm diameter. In this example, the threshold of motion is exceeded for $\theta_{max}=0.043$, and the threshold of suspension for $\theta_{max}=0.214$.

Van Rijn (2007) presented empirical trend lines taken from a large data compilation for bedload and suspended transport rates under current-only river and tidal flow conditions. For grain sizes finer than 0.2mm the bedload contribution is always less than 10% of the suspended load. For grains in the range 0.2-0.4mm, this is also true for current speeds greater than $0.9ms^{-1}$, and for 0.4-0.6mm grains for currents $>1.3ms^{-1}$. Van Rijn comments that field data sets for combined current and wave conditions are rather scarce, and do not generally include bedload measurements. However, the effect of adding waves is analogous to increasing the current speed, so the limits for bedload being less than 10% of the total load for coarser grains will be reduced in the presence of waves. These observations are consistent with the switch-over of functions R_s and R_b shown in Figure 1b, since coarse grains correspond to small θ_{max} for given wave and current conditions.

Turbulent diffusion

Turbulent velocity motions generated by friction as seawater flows over the seabed impose quasi-random fluctuations on the motions of particles, which result in an initial tight cluster of particles taking different paths and diffusing into a cloud. The turbulent velocities of fluctuations are typically about 10-20% of the mean velocity, or more if waves are present (Soulsby and Humphery 1990).

Lagrangian models such as PLUME-RW cater for the turbulent diffusion of dissolved and fine suspended substances using the random walk method (Hunter 1987; Mead 1991, 2004; Mead and Rodger 1991). Model particles are subjected to random displacements in addition to the ordered movements that represent advection by mean currents. Provided the lengths of the turbulent displacements are correctly chosen, the random step procedure is analogous to the use of turbulent diffusivities in advection-diffusion models (Hunter 1987; Mead 2004). The displacement of a particle in each of the orthogonal horizontal directions is calculated from a Gaussian distribution, with zero mean and a variance determined from the specified horizontal diffusivity. The relationship between the standard deviation of the turbulent horizontal displacement, Δ, the timestep, Δt, and the diffusivity, D, is:

$$D = \Delta^2 / 2\Delta t \qquad (12)$$

In a PLUME-RW simulation, a horizontal diffusivity is specified, which the model reduces to turbulent displacements using Equation (12). Turbulent diffusion in SandTrack is implemented by first calculating the turbulent horizontal displacements during each timestep of the model using Equation (12). A value of the horizontal diffusivity of $D=0.2\text{m}^2\text{s}^{-1}$ is often used, since this has been found to be typical of values in coastal locations (for example, Elliott et al 1997). As with the deterministic advective movement, the diffusive motion of sand grains and industrial particles can be much slower than that of the seawater, being controlled by the F, P and R functions discussed previously. The distances (ℓ_x, ℓ_y) moved as a result of both advection and diffusion in the x and y horizontal directions by a tagged particle during a timestep of the model are therefore given by:

$$(\ell_x, \ell_y) = \text{F.P.R.}[(U_{xc}, U_{yc})\Delta t + (\Delta_x, \Delta_y)] \qquad (13)$$

where (U_{xc}, U_{yc}) are the orthogonal horizontal components of $\underset{\sim}{U}_c$, and (Δ_x, Δ_y) are the randomly-determined displacements (Equation (12)) due to turbulent diffusion in the same coordinate system.

Although turbulent diffusion is included in SandTrack for completeness of physical processes, in practice this fine-scale diffusion, operating at length-scales of a few metres and timescales of a few seconds, has only a small effect on the long-term distributions of the particles. The much larger spatial and temporal effects of including wind-induced deterministic water motions have much greater effects on the long-term distributions. This is expected from standard turbulent diffusion theory, which states that, for large diffusion times, only the long-period eddies contribute to the value of the eddy diffusivity (for example, Hinze 1959).

Wind-driven dispersion

SandTrack includes wind-driven velocity components in its grain movements. Constant or time-varying wind speeds and directions can be specified as input data and, in each model timestep, these are resolved into long-shore and cross-shore components. Model particles are allocated site-specific long- and cross-shore velocity increments, based on the prevailing wind speed, which have both ordered and random components. Further details of the components used in the Dounreay application were given by Soulsby et al (2006).

Wave-induced sediment transport

Waves drive sediment in the direction of wave travel by two mechanisms (FD92):

a) Wave asymmetry, in which the strong onshore velocity under the wave crest moves more sediment than the weak offshore velocity under the wave trough.

b) Mass transport, otherwise known as boundary-layer streaming, in which the vertical orbital wave motions near the seabed carry sediment up into strong onshore velocities in the upper part of the wave boundary layer, and down into weak offshore movements nearer the bed.

In SandTrack, these mechanisms are implemented through the inclusion of step-lengths added vectorially to the particle step-lengths in each model timestep calculated as described in this paper. The "asymmetry" step-lengths are based on an expression, related to second-order Stokes wave theory, derived to predict the magnitude of the velocity asymmetry as a function of significant wave height, the equivalent monochromatic wave period, and the water depth. In the interest of brevity, details of the derivation of this expression are not given here. The total bedload transport rate due to both a) and b) above is taken to be that for wave asymmetry alone multiplied by a factor derived from the analysis of Myrhaug et al (2004).

Constants

Values for various constants are calculated at the start of a SandTrack simulation. They depend on the water temperature and salinity, the tagged and indigenous particle diameters (d_t and d_a respectively), and the tagged and indigenous particle densities ($\rho_{s,t}$ and $\rho_{s,a}$ respectively). The calculations are based on information presented in DMS on water density, ρ (Figure 2 of DMS) and kinematic viscosity, ν (Figure 3 of DMS), plus equations for the threshold Shields parameter, θ_{cr}, and particle settling velocity, w_s, also taken from DMS:

$$\theta_{cr} = \frac{0.30}{1+1.2D_*} + 0.055\left[1-\exp\left(-0.020D_*\right)\right] \tag{14}$$

$$w_s = \frac{\nu}{d}\left[\left(10.36^2 + 1.049D_*^3\right)^{1/2} - 10.36\right] \tag{15}$$

where $D_*=(g(s-1)/\nu^2)^{1/3}d$ is the non-dimensional grain size, g is the acceleration due to gravity and $s=\rho_s/\rho$. θ_{cr} is a non-dimensional measure of the shear stress generated at the seabed by currents and waves that is just sufficient to move a particle that is resting on a flat bed of particles identical to itself. A correction, via a hiding/exposure function, must be applied to θ_{cr} to take account of a tagged grain being a different size to the natural seabed grains on which it rests. For the purpose of deriving this function, the mobile tagged grain is assumed to sit on the surface of the indigenous grains of the seabed, rather than within the near-surface mobile layer of the bed. Solid geometry considerations that account for (a) the reduced friction angle, and (b) the increased exposed surface area of the tagged grain if it is larger than the bed grains (and vice versa if it is smaller), lead to an expression for the threshold Shields parameter of the tagged grain, $\theta_{cr,A}$:

$$\frac{\theta_{cr,A}}{\theta_{cr}} = \left(\frac{8}{3A^2+6A-1}\right)^{1/2} \cdot \frac{3.2660A}{\left[4A-2\left\{A+1-\left(A^2+2A-1/3\right)^{1/2}\right\}\right]} \tag{16}$$

where $A=d_t/d_a$ is the ratio of the tagged to indigenous grain diameters. The full derivation of Equation (16) is given by Soulsby (2010). The equation yields a dependence on A similar in form to that obtained by other researchers on the basis of different assumptions (Egiazaroff 1965; Ribberink 1987). If the tagged grain is the same size as the natural bed, then A=1 and

$\theta_{cr,A}=\theta_{cr}$. However, for a tagged grain of, for example, diameter 2mm lying on a bed of grains of diameter 0.25mm, A=8 and $\theta_{cr,A}=0.1546\theta_{cr}$. This greatly increases the grain's mobility compared with the uncorrected case. For A<0.155, the tagged grain can fall through the matrix of bed grains, and is consequently treated as being immobile.

Near-bottom current speed, U_c

In SandTrack, the velocities computed by the flow model are used to calculate U_c as the current velocity averaged over the lowest 1m layer of the water column, at the horizontal position of each model particle. This derivation uses the one-seventh power law velocity profile, based on a wide range of observed current velocity profiles and presented in DMS.

Wave orbital velocity

Both the significant wave height, H_s, and the wave zero-crossing period, T_z, vary with time according to the varying wind-speed throughout a SandTrack run. The waves are assumed to conform to a JONSWAP spectrum, which is typical of waves in relatively shallow water (that is, at depths shallow enough for wave action to penetrate significantly to the seabed). The root-mean-square (RMS) orbital velocity at the seabed produced by a combination of all the wave frequencies in the spectrum is calculated from H_s, T_z and water depth using a formula from DMS, Soulsby and Smallman (1986) or Soulsby (1987). An "equivalent monochromatic wave" is defined, so as to make use of established methods for calculating bed shear stresses and sediment movement. This is taken to be the sinusoidal wave whose period is equal to the period at the peak energy in the spectrum, and which has an RMS velocity equal to that of the full spectrum of waves.

Bed shear stress

Wave-induced and tidal velocities combine non-linearly to produce time-varying bed shear stresses, which can be characterised at a given point by the mean bed shear stress (τ_m) and the maximum bed shear stress (τ_{max}) during a wave period, T. Related quantities are friction velocities (u_{*m}, u_{*max}, where $u_*=\sqrt{(\tau/\rho)}$) and Shields parameters (θ_m, θ_{max}, where $\theta=\tau/(g(\rho_s-\rho)d)$). In SandTrack, τ_m and τ_{max} are calculated from the bed shear stresses due to currents alone and waves alone, τ_c and τ_w respectively, using the following equations from DMS:

$$\tau_m = \tau_c \left[1 + 1.2 \left(\frac{\tau_w}{\tau_c + \tau_w} \right)^{3.2} \right] \tag{17}$$

$$\tau_{max} = \left[\left(\tau_m + \tau_w \left| \cos \phi \right| \right)^2 + \left(\tau_w \left| \sin \phi \right| \right)^2 \right]^{1/2} \tag{18}$$

where φ is the angle between current direction and direction of wave travel.

Test simulations

Tests of the model were made with the dual purpose of calibrating some free parameters, and checking whether the results were broadly in agreement with observations. This was achieved firstly by using it to simulate the distribution of natural sand in the coastal waters near Dounreay and, secondly, using the results of a number of particle surveys in the area.

Simulation of the natural sand distribution

Simulations of the natural sand distribution in the Dounreay coastal waters were carried out for various formulations of the wave asymmetry drift. Comparisons of the results of these tests with the known natural sand distribution showed that the theoretical drift expression gave the best agreement, without any additional tuning. Only the results of the test with the finalised wave asymmetry drift are presented and discussed here.

The simulations of the natural sand distribution were undertaken by initialising SandTrack with 1000 model particles positioned randomly across the computational domain, regardless of whether the bed type is sandy or rock/gravel. A random, rather than regular, initial distribution was chosen to be in keeping with the stochastic nature of the model, although the initial distribution rapidly becomes unimportant once the particles start moving. The particles had diameters of 0.25mm, typical of the indigenous sand in the area. As this set of tests investigated the behaviour of indigenous sand, trapping processes were omitted to represent the constant availability of grains to be transported. Figure 2 shows a comparison of the areas known from observations to be sandy or rock/gravel with the model particles after three years of simulated time.

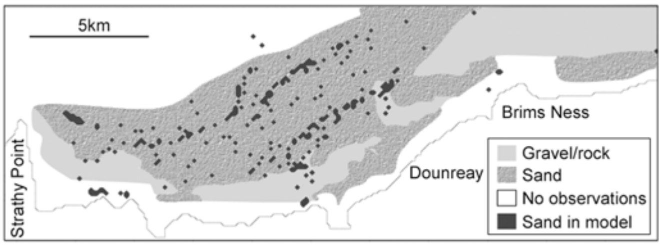

Figure 2. Comparison of sandy and rock/gravel areas with model particle locations after three years

The test results show clusters of particles in areas where the seabed sediment is known to be sandy. Areas known to consist largely of gravel lost most of the model sand particles initially seeded there after a few months. Around half of the model particles moved towards the northeast, past Brims Ness, where they passed through the eastern model boundary. In general, particles moved inshore, then towards the northeast in shallower water.

These results demonstrate that the calibrated model has the correct behavioural tendencies, and indicate, in particular, that the balance between the cross-shore drift associated with wave-induced transport and wind-induced currents is correct.

Simulations using particle survey results

A set of model simulations made use of existing results from periodic surveys carried out by UKAEA at four circular sites in the coastal waters near Dounreay, with the aim of establishing the mobility of the particles. Within these “repopulation areas”, any industrial particles found were recorded and removed at various times over a three-year period. Between surveys, these areas became repopulated with industrial particles by the natural tide, wave and wind processes. Each survey was split into two zones (inner and outer) demarcated by two concentric circles with radii of 28.2m and 50.0m. Comparisons between the model results and the repopulation data were used to determine whether the model was simulating the actual rates of repopulation in the field. In turn, this indicated whether the model was reproducing correctly the effects of the grain trapping and transport processes.

The simulations included tuning of the trapping algorithm parameters, using data for one of the four repopulation areas. For each repopulation area, SandTrack was driven with time series of wave and current conditions appropriate to that area, over the whole three-year period. Wind and wave data were taken from the UKMO European Wave Model, and flow conditions were taken from a three-dimensional tidal hydrodynamic model of the area. In each case, SandTrack was initialised with model particles distributed at random using a particle distribution density based on the field data. The model was run over the three-year period of the field surveys and, at times corresponding to each specific survey, the number of model particles in each repopulation area was recorded and the particles were removed.

Initially, the trapping algorithm parameters were adjusted during sensitivity testing. The parameters adjusted were the initial proportion of particles free, the equilibrium proportion of particles free, γ_e, the transition scale value, θ_s, and the maximum transition probability per second, b_e. The optimum parameter set, for which results are presented here, was $\gamma_e=0.1$, $\theta_s=0.1$, and $b_e=1.7\text{x}10^{-7}\text{s}^{-1}$. In all of the simulations discussed in this paper, a timestep of 20 minutes was used, to correspond with the available driving wave and current data.

The numbers of actual and simulated particles recovered for the repopulation area with the most repeat surveys have been discussed by Soulsby et al (2006), and are not considered further here. The results for all four areas together are summarised in Figure 3. It is noted that both the model predictions and the natural particle movements result from stochastic processes, and therefore some variability in the level of agreement between the model and the observed data is to be expected. This is compounded by the fact that the numbers of particles being dealt with were small, especially in Figure 3a (less than 15 particles). The predicted numbers of particles lie within a factor of two of the observed numbers for 52% of cases in the inner areas (Figure 3a), and for 75% of cases in the outer areas (Figure 3b). Sediment predictions in coastal conditions rarely exceed 70% of predictions lying within a factor of two of observations (Van Rijn 2007). Where the number of particles is statistically sufficient (Figure 3b), the level of agreement is therefore acceptable, and the larger scatter in Figure 3a is also acceptable given the effects of stochasticity on small numbers.

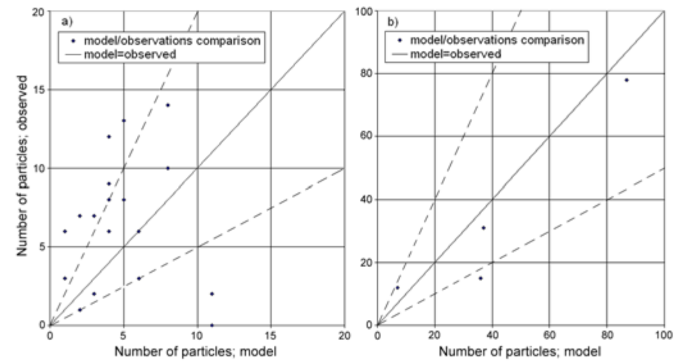

Figure 3. Comparison of actual and simulated particle numbers recovered for all the repopulation areas: (a) inner areas, and (b) outer areas; dashed lines show the envelope of factor-of-two agreement

Predictive simulations

The results of simulations of the movement of Dounreay industrial particles are presented here, for representative particle sizes of 0.25mm, 0.5mm, 1.0mm and 2.0mm. In these simulations, particle release took place over a period of a few days in the late 1960s, at a point source, representing the diffuser structure on the Dounreay outfall, some 300m from the shore. The simulated distributions of particles after 30 years are shown for the four particle sizes in Figure 4.

Figure 4 indicates that the long-term distribution of particles was strongly dependent on particle size. A majority of particles moved towards the northeast model boundary for all grain sizes, but the smaller grains travelled further west than the larger grains. Particles which moved to the west tended to collect at the centre of the residual eddies to the east and west of Strathy Point. Similar hydrodynamic features exist to the east and west of Brims Ness, and particle accumulations in these areas are also evident in Figure 4. Most of the 2.0mm particles were to the northeast of the diffuser after 30 years. Many processes which depend on particle size are represented in SandTrack, but the most likely reason for the different behaviour of the different sizes is the lower threshold of motion, and of suspension, of the finer sizes. They will thus be mobile for a greater proportion of the time and hence disperse further, whereas the coarsest particles move mainly as bedload, and only at the times of the largest waves and currents.

Figure 5b shows the model particle positions, for the four particle sizes together, at the end of the 30-year simulations, compared with the actual recovered particle locations over a 10-year survey period in Figure 5a. Recoveries could only be made in relatively shallow water, so the model results cover a greater area than the observations. The model is broadly in agreement with the field data, with recovered particles being found mainly within the envelope of model particle locations, including the margins of Sandside Bay.

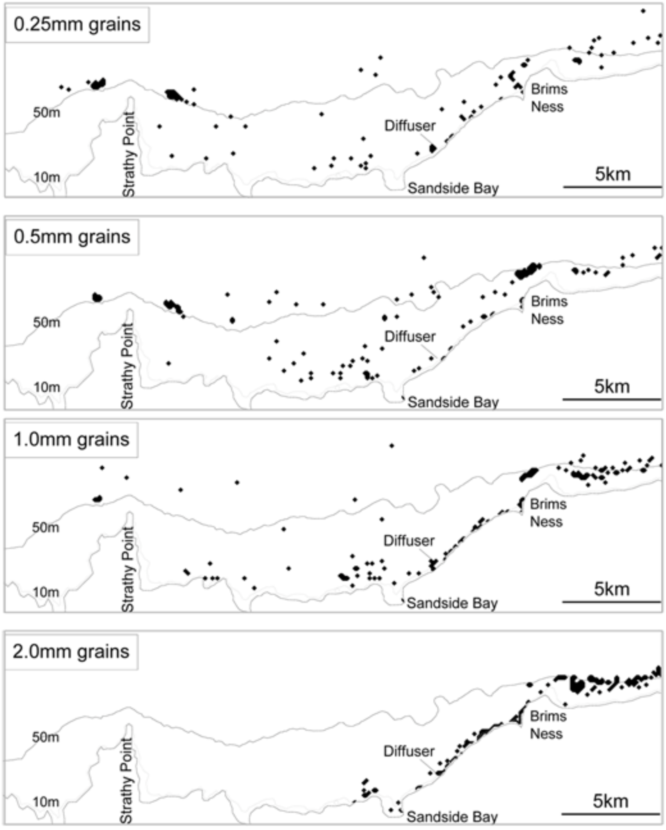

Figure 4. Particle distributions after 30 years in the predictive simulations (reprinted from Soulsby et al (2006), with permission from the MWWD Organisation)

Figure 5 indicates that both the model results and actual particle recoveries in the field showed some particles in the vicinity of the diffuser after several decades. This was a complex feature of the field recoveries which early versions of SandTrack did not reproduce, due to the relative simplicity of the particle trapping algorithm at that time. Those models tended to move particles away from the diffuser, both eastwards and westwards, so that none remained within 2km of the diffuser after 20 years. The trapping algorithm represented by Equations (2) to (5) overcame this difficulty, together with the tuning of the model using the repopulation data described previously, by introducing a distribution of particle residence times within the seabed consistent with the available data.

Conclusions

A model, SandTrack, has been established to simulate movements of sand-sized particles, or tagged particles, within a Lagrangian framework. The model can be applied to assess the dispersal of contaminated particulate material, such as may be associated with industrial discharges, or the dispersal of dredged spoil.

SandTrack has been tested for the coastal waters near Dounreay, against (a) field observations of natural sand, (b) surveys of the re-population of given areas after they have been cleared of contaminated industrial particles, and (c) the observed overall distribution of contaminated particles in the Dounreay area. The tests showed broad agreement with expected trends, and the limited observations available. They have strengthened confidence in SandTrack predictions, and have enabled appropriate values of some of the model's main physical parameters to be set. Of particular note, is the model's reproduction of particle recoveries near the diffuser several decades after their release, which was not achievable with simpler models. Predictive simulations carried out for periods of 30 years have elucidated long-term particle behaviour, such as tendencies to accumulate at the centres of residual eddies adjacent to headlands, and for fine particles to be dispersed both east and west of the diffuser but for coarse particles to travel predominantly east at this site.

A 30-year SandTrack simulation with a 20-minute timestep can be completed in significantly less than 24 hours, so the model is a reasonably practical tool for assessing long-term particle dispersal.

Acknowledgements

The development of the SandTrack model was carried out under contract to UKAEA, whose permission to publish the model results here is acknowledged gratefully

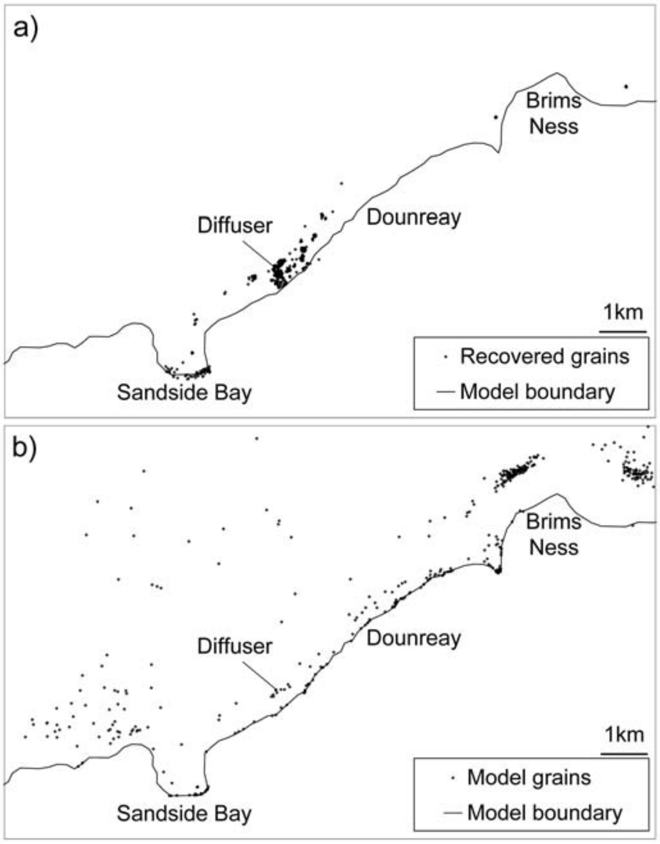

Figure 5. (a) actual recovered particle locations over a 10-year survey period; and (b) model particle locations, for all simulated particle sizes, after 30 years in the predictive simulations

Notation

The following symbols are used in this paper:

A = ratio of tagged grain diameter to the diameter of the grains of the bed;
a, b = probabilities of a trapped/free grain becoming free/trapped;
B = $w_s/(0.4u_{max})$;
b_e = maximum free-to-trapped transition probability in a second;
C = concentration;
D = horizontal diffusivity;
D_* = non-dimensional grain size;
d_t, d_a = tagged, indigenous grain diameters;
F = freedom factor;
g = acceleration due to gravity;
H_s = significant wave height;
ℓ_x, ℓ_y = x, y distances moved by a tagged grain during a timestep;
P = probability that a free grain is moving;
R = reduction factor for the speed of a mobile grain;
R_b, R_s = reduction factors for bedload and suspended load;
s = ratio of grain and water densities;
T = wave period;
T_z = wave zero-crossing period;
U = horizontal current speed;

U_b = horizontal speed of a grain undergoing bedload transport;

U_c = horizontal current speed averaged over the lowest 1m of the water column;

U_{gr} = horizontal speed of a mobile grain;

U_s = weighted-mean horizontal speed of suspended grains;

U_{xc}, U_{yc} = x, y components of U_c;

u_{*m}, u_{*max} = mean, maximum horizontal friction velocities;

w_s = settling velocity;

x, y, z = Cartesian coordinates;

z_1, z_2 = heights of the bedload layer and the upper limit for suspended transport;

γ = proportion of particles that are free;

γ_e = equilibrium proportion of particles that are free;

Δ = turbulent horizontal displacement in a model timestep;

Δ_x, Δ_y = x, y components of Δ;

Δt = model timestep;

θ_{cr} = threshold non-dimensional bed shear stress for a grain lying on a flat bed of grains identical to itself;

$\theta_{cr,A}$ = threshold non-dimensional bed shear stress for a tagged grain lying on a flat bed of particles different from itself;

$\theta_{cr,a}$, $\theta_{max,a}$ = values of θ_{cr}, θ_{max} for indigenous sediment grains;

θ_m, θ_{max} = mean, maximum Shields parameters over a wave cycle;

θ_s = scale value which determines the distribution of tagged grain residence times in the seabed;

μ_d = dynamic friction coefficient;

ν = kinematic viscosity;

ρ = water density;

$\rho_{s,t}$, $\rho_{s,a}$ = tagged, indigenous grain densities;

τ_c, τ_w = current-only, wave-only bed shear stresses;

τ_m, τ_{max} = mean, maximum bed shear stresses over a wave cycle; and

φ = angle between current and wave directions.

References

Egiazaroff, I.V. (1965). “Calculation of non-uniform sediment concentration.” *J. Hydraulics Div., ASCE,* 91(HY4), 225-248.

Elliott, A. J., Barr, A. G., and Kennan, D. (1997). “Diffusion in Irish coastal waters.” *Estuarine, Coastal and Shelf Science*, 44A, 15-23.

Engelund, F., and Fredsøe, J. (1976). “A sediment transport model for straight alluvial channels.” *Nordic Hyrdology*, 7, 293-306.

Fredsøe, J., and Deigaard, R. (1992). *Mechanics of Coastal Sediment Transport*, World Scientific Publishing Co., Singapore.

Gailani, J. Z., Lackey, T. C., and Smith, J. (2007). “Application of the Particle Tracking Model to predict far-field fate of sediment suspended by nearshore dredging and placement at Brunswick, Georgia.” *Proc. XVIII World Dredging Congress 2007*, WEDA, Lake Buena Vista, Florida, USA, 1359-1375.

Hinze, J.O. (1959). *Turbulence,* McGraw-Hill Book Company Inc, New York.

Hunter, J. R. (1987). “The application of Langrangian particle-tracking techniques to modelling of dispersion in the sea.” *Numerical modelling: applications to marine systems*, Elsevier Science Publishers B V, North Holland, 257-269.

Lackey, T. C., and MacDonald, N.J. (2007). “The Particle Tracking Model: description and processes.” *Proc. XVIII World Dredging Congress 2007*, WEDA, Lake Buena Vista, Florida, USA, 551-565.

MacDonald, N. J., and Davies, M. H. (2006). "Particle-based sediment transport modelling." *Proc., 30th Int. Conf. on Coastal Engineering*, ASCE, San Diego, 3117-3128.

Madsen, O.S. (1991). "Mechanics of cohesionless sediment transport in coastal waters." *Proc., Coastal Sediments '91*, ASCE, New York, 15-27.

Mead, C. T. (1991). "Random walk simulations of the dispersal of sewage effluent and dredged spoil." *Proc., 10th Australasian Conf. on Coastal and Ocean Engineering*, Auckland, New Zealand, 477-480.

Mead, C. T. (2004). "Realisation of the potential of Lagrangian models in aquatic dispersion studies". *Proc., 3rd Int. Conf. on Marine Waste Water Disposal and Marine Environment*, Catania, Italy.

Mead, C. T., and Rodger, J. G. (1991). "Random walk simulations of the dispersal of dredged spoil." *Proc., Int. Symp. on Environmental Hydraulics*, Hong Kong, 783-788.

Myrhaug, D., Holmedal, L. E., and Rue, H. (2004). "Bottom friction and bedload sediment transport caused by boundary layer streaming beneath random waves." *Applied Ocean Research*, 26, 183-197.

Ribberink, J.S. (1987). "Mathematical modelling of one-dimensional morphological changes in rivers with non-uniform sediment." Thesis, Univ. of Technology Delft, Delft, The Netherlands.

Soulsby, R.L. (1987). "Calculating bottom orbital velocity beneath waves." *Coastal Engineering*, 11, 371-380.

Soulsby, R. L. (1997). *Dynamics of Marine Sands: a Manual for Practical Applications*, Thomas Telford Publications, London.

Soulsby, R. L. (2010). "Threshold of motion of bimodal sand sizes in the SandTrack model. A new hiding/exposure function." HR Wallingford Report TR190.

Soulsby, R. L., and Humphery, J. D. (1990). "Field observations of wave-current interaction at the sea bed." *Water Wave Kinematics,* Kluwer Academic Publishers, The Netherlands, 413-428.

Soulsby, R. L., and Smallman, J. V. (1986). "A direct method of calculating bottom orbital velocity under waves." HR Wallingford Report SR76.

Soulsby, R. L., Mead, C. T., Wild, B. R., and Wood, M. J. (2006). "A model for simulating the dispersal tracks of sand-sized particles in coastal areas – 'SandTrack'." *Proc., 4th Int. Conf. on Marine Waste Water Disposal and Marine Environment*, Antalya, Turkey.

Soulsby, R. L., Mead, C. T., and Wild, B. R. (2007). "A model for simulating the dispersal tracks of sand grains in coastal areas – 'SandTrack'." *Coastal and Shelf Sediment Transport. Geological Society Special Publications*, 274, 65-72.

Spearman, J., Bray, R. N., Land, J., Burt, T. N., Mead, C. T. and Scott, D. (2006), "Plume dispersion modelling using dynamic representation of trailer dredger source terms." *Proc., 7th Int. Conf. on Nearshore and Estuarine Cohesive Sediment Transport Processes*, Gloucester Point, Virginia, USA.

Van Rijn, L.C. (2007). "Unified view of sediment transport by currents and waves. II: suspended transport." *J. Hydraulic Engineering*, 133, 668-689.