MIKE 21 & MIKE 3 Flow Model FM

Particle Tracking Module

Scientific Documentation

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PLEASE NOTE

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APPENDICES

1 Introduction to Particle Tracking

Particle tracking techniques can be an efficient way to study fate of matter in the water environment. This technique uses a Lagrange discretization, splitting all mass in the system into a number of particles with specific 3D coordinates and masses, instead of the alternative Euler discretization, in which mass is represented as average concentrations in the computational mesh.

The basic idea behind particle tracking is to transport particles according to a drift regime, and adding dispersion by introducing a random walk term.

The performance of the particle tracking model depends directly on the number of particles in the domain, thus a problem can be solved quickly if the mass in the domain is only split into a few particles, and the same problem will be solved slower if the mass is split into many particles.

Particle tracking is an appealing approach to study narrow plumes of matter, because the simulated width of the plume is independent of the resolution of the computational mesh, whereas with the Euler approach the plume cannot be narrower than the resolution of the mesh.

Another advantage of particle tracking is that the Lagrangian approach has negligible numerical diffusion.

The Particle Tracking Module is also suitable for simulating particle tracks and following trajectories in the water environment. Additional drift from wind in the surface affecting the surface tracers can also be simulated.

Besides the basic processes with drift and dispersion, the functionality has been expanded with extra processes: settling, buoyancy, and erosion. These processes can be important for simulating particles with other densities than water, such as mud and sand. Furthermore, decay has been included for simulating non-conservative matter, as for instance coliform bacteria or other organic material.

1.1 Model Simplifications

The particle tracking model is a simplification of the real world, and the user should be aware of some of the simplifications:

1. It uses a Lagrangian discrete parcels method neglecting the interaction between diffusing particles. This means that Fick's dispersion law is not considered, and this is a reasonable assumption when discharging particles into systems with few other particles. A situation where this simplification could be a problem would be if particles where distributed homogeneously in a stream with larger diffusivity in the middle of the stream than on the sides. The particle tracking dispersion would then make a nonhomogeneous distribution with more particles on the sides than in the middle of the stream, which should not be physically possible according to Fick’s law.

2. Instant acceleration is assumed and therefore the particles have velocities according to the surrounding water flow. This is a physical simplification only possible for particles with zero mass, but since the masses considered in the Particle Tracking

Module usually are so small that the acceleration is almost instant the error is insignificant. If the particles were very heavy, the error would be significant.

1.2 Langevin Equation

The Particle tracking technique describing transport and dispersion of particles follows the Langevin equation. According to Einstein's explanation of observed Brownian motion during the first decade of this century, attempts were made by Langevin and others to formulate the dynamics of such motions in terms of stochastic differential equations. The resulting equations were written as

$$dX_t = a(t, X_t)dt + b(t, X_t)\xi_t dt \tag{1.1}$$

Where:

a	Drift term
b	Diffusion term
ξ	Random number

To simulate a trajectory of the Euler approximation Y for a given time discretization we simply start from the initial value $Y_0 = X_0$ and proceed recursively to generate the next value.

$$Y_{n+1} = Y_n + a(t, X_t)Y_n\Delta_n + b(t, X_t)Y_n\Delta W_n \tag{1.2}$$

For $n = 1,\ \ 2,\ \ 3,\ \ ....$ according to the Euler scheme with drift a and diffusion coefficient b.

Here $\Delta W_n = W_t - W_s \in N(\mu = 0, \sigma^2 = \Delta_n)$ is the normal distributed Gaussian increment of the Wiener process W, which is a continuous-time Gaussian stochastic process with independent increments over the subinterval $\tau_n \le t \le \tau_{n+1}$.

1.3 Classes

The particles in the Particle Tracking Module are divided into different groups called classes. Each class has specific properties regarding decay, settling/buoyancy, erosion, and dispersion, which have to be specified separately. In each class can also be specified a minimum mass and a maximum age of a particle.

These parameters are introduced in order to exclude particles that have died, or have decayed to insignificant masses, and thereby to increase the computational performance which is proportional to the number of particles in the system.

Typical examples of classes are different size fractions of sediment particles, but it could also be different organic pollutants with different decay rates.

2 Drift

The combined effects of current, wind drag and bed drag cause the drift of the particles.

2.1 Drift from Current and Wind

The drift vector $\vec{a}$ in Equation (1.1) is normally varying in space, see Equation (2.1). It represents the combined effects of current and wind drag that cause the advection of the particles, see Figure 2.1.

$$\vec{a}(x,y,z,t) = f\left(current, wind\ drag, bed\ drag\right) \tag{2.1}$$

2.1.1 Horizontal variation

The horizontal variation in the drift vector $\vec{a}$ is normally calculated in the hydrodynamic simulation. However, in areas with wind induced currents at very deep water where the flow is not influenced by bed resistance, the horizontal drift variation can be estimated directly as function of the wind by using the theory for the Ekman spiral.

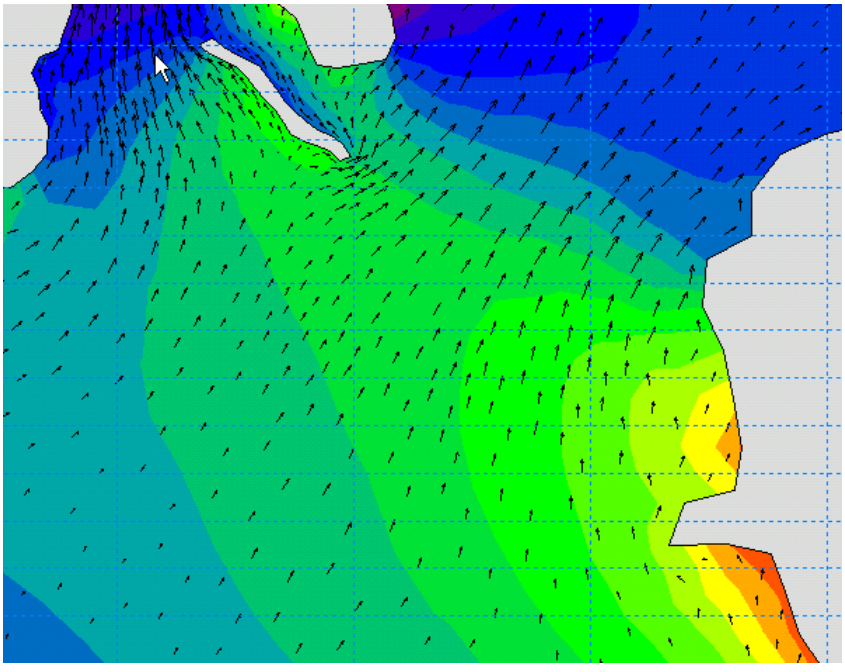

Figure 2.1 Example of Horizontal variation of Current drift

2.1.2 Vertical variation

The drift profile is a description of the vertical variation of the drift regime that influences the particles. It will normally be the currents and the wind that governs the shape of the drift profile. Currents and wind are already calculated in the hydrodynamic setup, but the hydrodynamic output does usually not have a fine discretization of the current profile near the bed. For MIKE 21 FM, for instance, it is the depth average values that are the output of the hydrodynamic setup, and even for MIKE 3 FM the drift conditions near the bed are normally not resolved adequately for describing sediment particles. Therefore it can be a good idea to assume some shapes of the vertical drift profile.

It is possible to include the bed friction drag in the current profile by assuming a bed shear profile (or logarithmic profile). For MIKE 21 FM the bed shear profile will be applied in the whole water column. In MIKE 3 FM it will only be applied in the bottom layer of the model, and the calculated flow conditions in the other layers will be used directly.

The wind drag can also cause increased flow velocities in the upper part of the water column, and corresponding velocities in the opposite direction in the lower part. In MIKE 3 FM this effect can be included in the hydrodynamic output, but the depth averaged MIKE 21 FM is not able to do that. So if this flow regime should be described in MIKE 21 FM PT, the wind induced profile must be applied, which will distribute the depth averaged flow in the water column.

If particles are in the water surface they can be influenced directly by the wind in addition to the influence from the flow. This will result in an additional acceleration of the particle in a direction relative to the wind turned with a wind drift angle caused by Coriolis forces.

2.2 Bed Shear Profile (Logarithmic Profile)

The vertical variation in the drift vector $\vec{a}$ is only calculated in 3D hydrodynamic simulations. The resolution of the vertical current profile is therefore dependent on the number of layers in the hydrodynamic simulation. The user has the option of modifying the drift profile with a logarithmic profile in the bottom layer of the 3D hydrodynamic current field to get a better description of the near bed conditions without having to use very fine vertical resolution.

In 2D hydrodynamic simulations with depth integrated current fields, the bed shear profile can be applied in the whole water column.

The shape of the velocity profile within a turbulent boundary layer is well established by both theory and experiment. The profile has specific characteristics very close to the bed where viscosity controls the vertical transport of momentum, and different characteristics farther from the bed where turbulence controls the vertical transport of momentum. The region closest to the bed boundary is called the laminar sub-layer or viscous sub-layer, because within the region turbulence is suppressed by viscosity. The viscous, laminar sub-layer only plays a significant role for smooth flows, where a typical thickness of the viscous layer is about 2 cm, whereas for rough flows the viscous sub layer is typically less than 1 mm and not included in the PT module, and instead the flow is set to zero for z smaller than z0, see Figure 2.2.

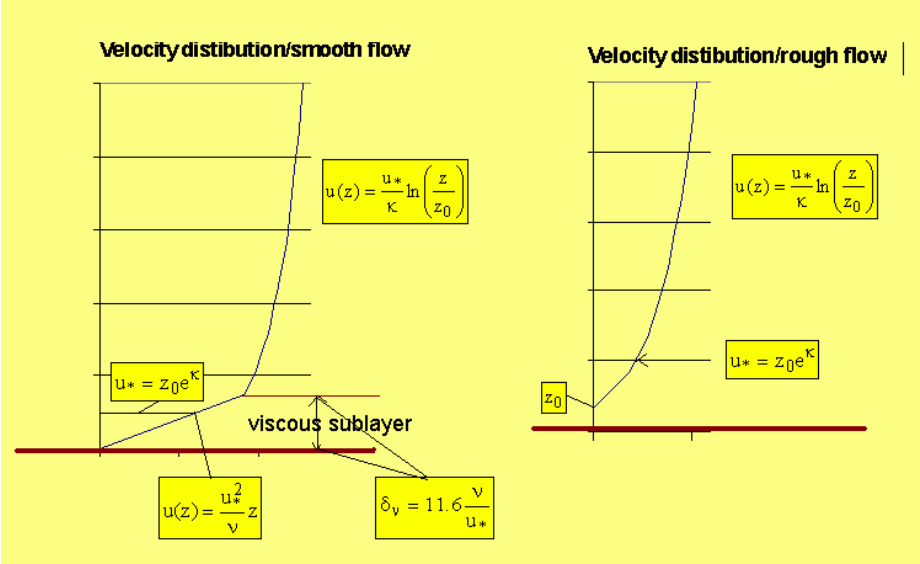

Figure 2.2 Example of bed shear profile applied from 2D flow fields

Logarithmic layer (z >= δ_v smooth flow**) (z >=** z0 rough flow**)**

$$u = \frac{2.3}{k} \cdot u^* \cdot \log_{10} \frac{z}{z_0} \tag{2.2}$$

Smooth flow: Laminar bed shear layer (z < δ_s**)**

$$u = \left(u^*\right)^2 \cdot \frac{z}{\nu} \tag{2.3}$$

Where:

κ	Von Karman empirical constant 0.4
z_0	Characteristic roughness
z	Coordinate from bed towards water surface [m]
u^*	Friction velocity, see Equation (2.4)
δ_v	Thickness of viscous bed shear layer
ν	Kinematic viscosity of water

2.2.1 Friction velocity

The friction velocity is used for estimating the bed shear profile, the viscous sub layer width, and to determine whether a flow is rough or smooth.

Friction velocity is defined as in Equation (2.4) and can be interpreted as the current velocity near the bottom. τ_{bed} is already calculated in the hydrodynamics of MIKE 21 FM and MIKE 3 FM, so the definition is used directly to estimate the friction velocity in the Particle Tracking Module.

$$u^* = \sqrt{\frac{\tau_{bed}}{\rho}} \tag{2.4}$$

Where:

τ_{bed}	Bed shear stress (calculated in the hydrodynamics)
ρ	Density of water

2.2.2 Characteristic roughness z0

The characteristic roughness is an important parameter for estimating the bed shear profile. It is estimated with different methods depending whether the flow is rough or smooth.

Roughness for smooth turbulent flow (Re < 5)

$$z0 = \frac{\nu}{9u^*} \tag{2.5}$$

Roughness for rough turbulent flow (Re > 70)

$$z0 = \frac{\varepsilon}{30} \tag{2.6}$$

Transitional flow, neither smooth nor rough turbulent flow (5 < Re < 70)

$$z0 = \frac{\nu}{9u^*} + \frac{\varepsilon}{30} \tag{2.7}$$

Where:

ν	Kinematic viscosity of water
ε	Nikuradse roughness
u^*	Friction velocity
Re	Reynolds number

$$\mathrm{Re} = \frac{u^* \varepsilon}{\nu} \tag{2.8}$$

2.2.3 Thickness of laminar sub-layer

$$\delta_v = \frac{11.6 \cdot \nu}{u^*} \tag{2.9}$$

Where:

ν	Kinematic viscosity of water, see **Error! Reference source not found.**
u^*	Friction velocity

2.3 Wind Induced Profile of Depth Integrated 2D Currents

The wind drag can also cause increased flow velocities in the upper part of the water column, and corresponding velocities in the opposite direction in the lower part. In MIKE 3 FM this effect can be included in the hydrodynamic output, but the depth averaged MIKE 21 FM is not able to do that. So if this flow regime should be described in MIKE 21 FM PT, a wind induced profile must be applied, which will distribute the depth averaged flow in the water column.

This has been done by calculating a wind drift vector that is multiplied with the current velocity vector, see Figure 2.3 and Figure 2.4.

The magnitude of the surface wind drift vector c_w^* is commonly assumed to be proportional to the magnitude of the wind speed 10 m above the sea surface. This factor c_w^* has a common value that varies from 0.01 to 0.06 (from *Al-Rabeh (1994)*).

The vertical distribution of the wind drift vector consists of an offshore part and an onshore part. The onshore distribution is based on a parabolic vertical profile and is able to produce backflow at depths, where the offshore logarithmic profile does not.

The parabolic profile acts in shallow waters with a water depth less than a specified water depth, h_{sep}, which is a positive value (in metres) and measured from the free water surface.

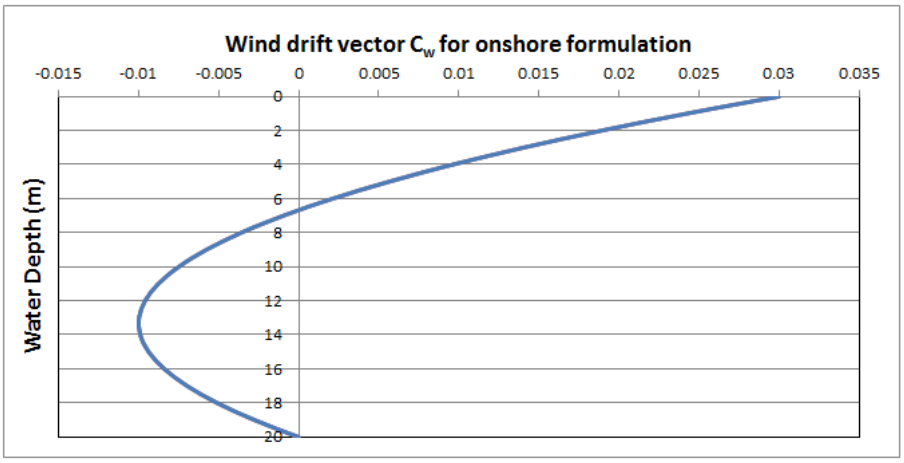

Figure 2.3 Onshore wind induced profile (2D currents) for a water depth = 20 m and a wind drift factor = 0.03

The vertical distribution of the parabolic onshore profile is given by

$$c_w(z) = c_w^* \left(1 - 3\frac{z}{h}\right)\left(1 - \frac{z}{h}\right) \qquad (2.10)$$

Where:

h	Local water depth in meter
z	Vertical particle co-ordinate, measured from sea surface
c_w^*	Wind drift factor (input)

The parabolic profile causes the wind-generated flow in the upper third of the water column to be in the same direction as the current and the flow in the lower part to be in the opposite direction of the wind. There is no net depth averaged mass transport due to the wind.

The vertical distribution of the offshore wind drift vector is given by

$$c_w(z) = c_w^* \exp\left(-k_0\, z\right) \tag{2.11}$$

Where:

k_0	$3/h_w$ [m^{-1}]
h_w	Depth of wind influence [m]
z	Vertical co-ordinate measured from sea surface
c_w^*	Wind drift factor [-]

In order not to create an additional mass flux caused by wind shear stress, the current profile is adjusted such as to have zero net flow. The contribution can be expressed as:

$$c_w(z) = -\frac{1}{h_w}\int_0^{h_w} c_w(z)\, dz + c_w(z) \tag{2.12}$$

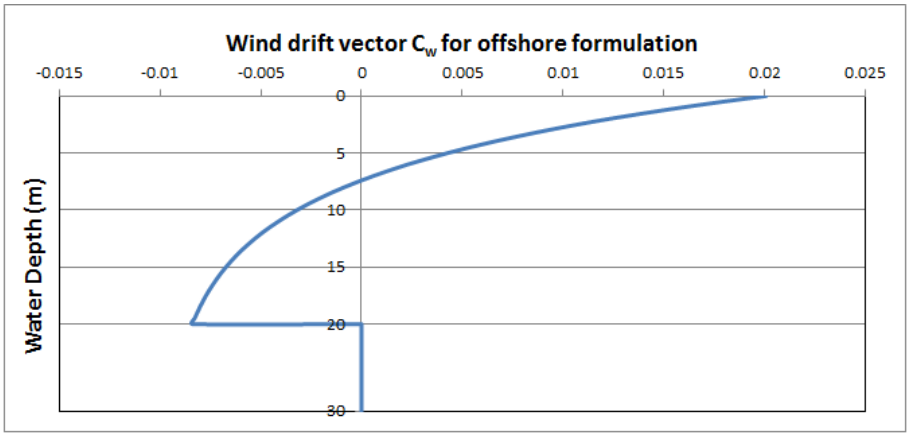

Figure 2.4 Offshore wind induced profile (2D currents) with h_w = 20m and the wind drift factor = 0.03

2.4 Wind Acceleration of Surface Particles

Particles that are exposed to wind in the water surface are affected according to the wind regime in 2 ways: indirectly via the currents that include the wind, but also directly as an extra force directly on the particle. How much of the wind speed that is transferred to the particle speed depends on the nature of the particle: how much is the particle exposed, etc.? Therefore, it is a calibration factor that expresses how much of the wind speed that is added to the particle speed.

In the Particle Tracking Module the wind acceleration of surface particles affect the drift with the following modification:

When the particle is in the top 5 cm of water column:

$$U_{particle} = U_{current} + windweigth \cdot W \cdot \sin\left(Winddirection - \pi + \theta_w\right) \quad (2.13)$$

$$V_{particle} = V_{current} + windweigth \cdot W \cdot \cos\left(Winddirection - \pi + \theta_w\right) \quad (2.14)$$

Where:

θ_w	Wind drift angle
windweight	Calibration factor for wind drag on particle

2.4.1 Wind drift angle

The Coriolis force is normally included in the hydrodynamic currents, but also for the wind acceleration of surface particles the Coriolis force must be considered.

Due to the influence from the Coriolis force, the direction of the wind drift vector is turned relatively to the wind direction. The angle θ_w of deviation is termed with the wind drift angle. It turns to the right on the Northern Hemisphere and to the left on the Southern Hemisphere. From *Al-Rabeh (1994)*, it is assumed that

$$\theta_w = \beta \exp\left(\frac{\alpha |U_w|^3}{g\gamma_w}\right) \quad (2.15)$$

Where:

α	$-0.3 \cdot 10^{-8}$
β	28^o 38'
γ_w	Kinematic viscosity ($m^2\ s^{-1}$)
g	Acceleration due to gravity ($m\ s^{-2}$)

The magnitude of the wind drift angle varies with the geographical location and wind speed and it is often estimated at 12-15 degrees in the North Sea.

3 Dispersion

In systems with still water or laminar flow the dispersion is a so-called molecular diffusion caused by Brownian motions of each molecule. In systems with turbulent flows the diffusion consists of both molecular diffusion and turbulent dispersion of which the turbulent part is normally by far the most important.

Numerical diffusion is negligible when using the Lagrangian discrete parcels method.

3.1 Reynolds Number

Whether a flow is laminar or turbulent depends of the relative importance of fluid friction (viscosity) and flow inertia. The ratio of inertial to viscous forces is the Reynolds number. Given the characteristic velocity scale, U, and length scale, L, for a system, the Reynolds number is

$$\mathrm{Re} = \frac{U \cdot L}{\nu} \tag{3.1}$$

Where ν is the kinematic viscosity of the fluid.

For most surface water systems the characteristic length scale is the basin-scale. Because this scale is typically large (1 m to 100 km's), most surface water systems are turbulent. In contrast, the characteristic length scale for groundwater systems is the pore scale, which is typically small, and groundwater flow is nearly always laminar.

3.1.1 Langevin equation

Both molecular and turbulent dispersion can be described by random walks using the Langevin equation

$$dX_t = a(t, X_t)dt + b(t, X_t)\xi_t dt \tag{3.2}$$

Where a is a drift term, b is a diffusion term, and ξ is a random number.

The molecular diffusion term is a function of temperature and the specie in question.

The turbulent dispersion term is a function of the flow conditions.
Sometimes the turbulent dispersion must also cover unresolved turbulence not resolved with the applied discretization.

3.2 Molecular Diffusion

3.2.1 Estimation of molecular diffusion coefficient

A simple estimate of the molecular diffusion coefficient *D* is obtained by using the Stokes-Einstein relation. The Stokes-Einstein relation asserts that the self-diffusion constant of a spherical particle immersed in a fluid is given by

$$D = \frac{kT}{6\pi\eta\rho} \tag{3.3}$$

Where:

k	Boltzmann constant
T	Absolute temperature
η	Viscosity of fluid
ρ	Radius of particle

Typical example of molecular dispersion coefficient *D*:

Dissolved oxygen in water: 2×10^{-5} cm^2/sec

Because the value of *D* is normally so small, molecular diffusion is much too slow to explain the actual vertical transport of oxygen and other substances in the water column in natural waters (except at very short distances).

3.3 Turbulent Dispersion

The dispersion observed in natural waters can instead be explained as being the result of turbulent dispersion. Turbulent dispersion is of great importance in natural waters.

3.3.1 Estimation of turbulent dispersion coefficient

The turbulent dispersion coefficient D can be specified as the eddy viscosity calculated in the hydrodynamic simulation, or it can be specified directly.

In coastal areas it is important to distinguish between horizontal dispersion, due to e.g. unresolved eddies, and vertical dispersion due to e.g. bed generated turbulence. Hence, dispersion in horizontal and vertical direction is specified separately.

3.4 Random Walk

The dispersion is described by the non-linear Langevin equation, see Equation (3.2), which is the base of random walk models.

The applied random walk method is a simple numerical solution to the Langevin equation. The stochastic differential equation is solved with an explicit Euler scheme:

$$\Delta x = x_n - x_{n-1} = A\left(x_{n-1,} t_{n-1}\right) \cdot \Delta t + \sigma_L \cdot N(0,1) \quad (3.4)$$

Where:

N(0,1)	Standard normal distribution ($\mu = 0, \sigma^2 = 1$)
σ_L	Standard deviation of turbulent dispersion

$$\sigma_L = \sqrt{2 \cdot \Delta t \cdot D_L} \quad (3.5)$$

D	Dispersion coefficient

4 Decay

To every particle a mass of the substance or particle class in question is attached. Unless it is a conservative particle class, the mass may be exposed to decay. First order decay is included:

$$\frac{dM}{dt} = -k \cdot M \tag{4.1}$$

Where:

M	Mass [kg]
k	Decay rate [s^{-1}]

Equation (4.2) is the included analytical solution of the first order decay given in Equation (4.1).

$$M(t) = M_o \exp\left(-k \cdot t\right) \tag{4.2}$$

Often the T_{90} value (time until 90 % has been decayed) can be found as a property for a particle class or a substance.

The T_{90} value [s] can be used to estimate the decay rate *k* with the following conversion:

$$k = \frac{\ln 10}{T_{90}} \tag{4.3}$$

The half life value T_{50} [s] can be used to estimate the decay rate *k* with the following conversion:

$$k = \frac{\ln 2}{T_{50}} \tag{4.4}$$

Please note that negative values for *k* will result in growth of the particle mass.

For growing particles a given doubling time $T_{doubling}$ [s] can be used to estimate the corresponding 'decay' rate *k* with the following conversion:

$$k = \frac{\ln 0.5}{T_{doubling}} \tag{4.5}$$

5 Settling

The user must specify fall or buoyancy velocities for each particle class (positive value for fall velocity and negative value for buoyancy velocity). The velocity that should be specified for each particle class is a measure of the velocity of one particle grain not affected by any neighbouring particles, because the velocity can be very dependent on the neighbouring particles, see Figure 5.1.

The effect of any neighbouring particles on settling can be included by including the option for flocculation modification and the hindered settling modification of the settling velocity, see Figure 5.3 and Figure 5.4.

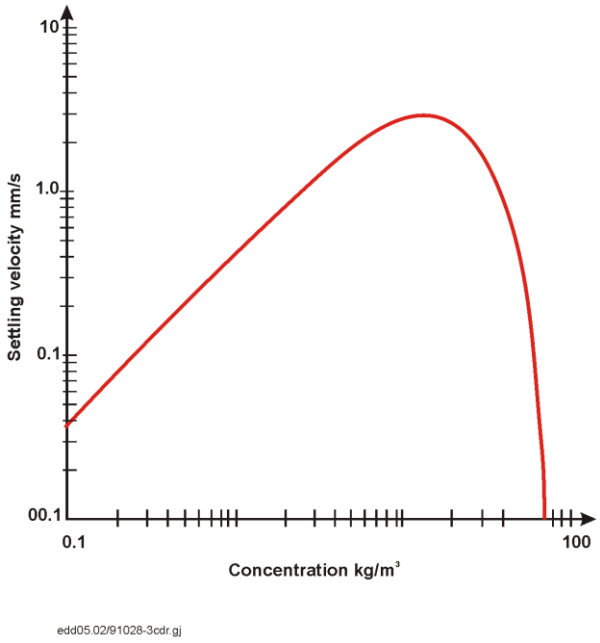

Figure 5.1 Typical settling velocity variation for mud

5.1 Stokes Law

When a sphere begins to move through a fluid, it accelerates and eventually reaches a constant velocity, called the terminal velocity. The terminal velocity is dependent on the particle size and described in Stokes' Law, which can be used as a rough estimate if no actual measurements are available of the particles. See examples of settling velocities and particle diameters in Figure 5.2.

$$w_s = \frac{(\rho_s - \rho) \cdot g \cdot d^2}{18\mu} \tag{5.1}$$

Where:

w_s	Particle fall velocity [m/s]
ρ_s	Sediment density [kg/m^3] (Quartz = 2650 kg/m^3)
ρ	Density of water [kg/m^3]

g Gravity : 9.81 m/s^2
d Diameter of particle [m]
μ Dynamic viscosity of water, see **Error! Reference source not found.**

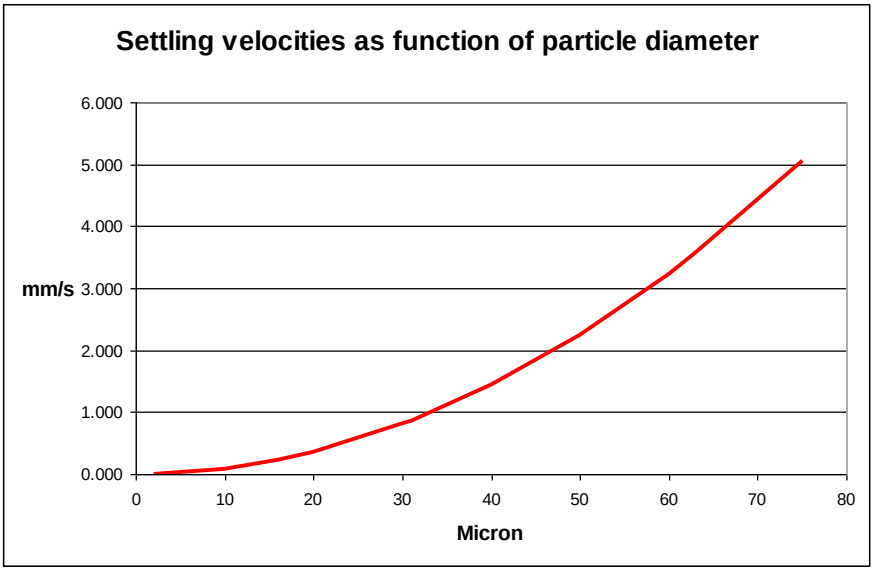

Figure 5.2 Relation between unflocculated settling velocities and particle diameter based on Stokes law

5.2 Flocculation

In case of fine grained cohesive sediment (<0.006 mm), the size of the particles and thereby the settling velocity will depend on the rate of flocculation.

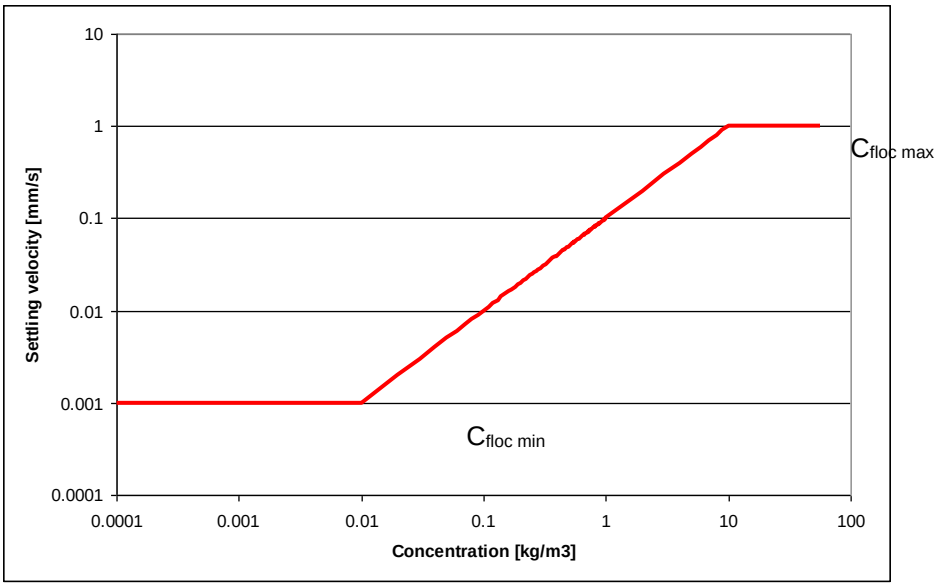

Figure 5.3 The principle of flocculation where the settling velocity is varying with total concentration

With low concentrations of suspended sediment, the probability of collision between the cohesive particles is low and the settling velocity will be close to the settling velocity for a single grain. With increasing concentration, collision between particles will occur more frequently and the cohesiveness of the particles will result in formation of flocs. This leads to an increase in average particle/floc size and hereby an increase in settling velocity. See Figure 5.3

$$w_s = w_0 \cdot factor_{floc} \tag{5.2}$$

$C_{total} <= C_{floc\ min}$:

$$factor_{floc} = 1 \tag{5.3}$$

$C_{floc\ min} < C_{total} < C_{floc\ max}$:

$$factor_{floc} = 1 + \alpha \left(\frac{C_{total}}{C_{floc\min}} - 1 \right) \tag{5.4}$$

$C_{total} >= C_{floc\ max}$:

$$factor_{floc} = 1 + \alpha \left(\frac{C_{floc\max}}{C_{floc\min}} - 1 \right) \tag{5.5}$$

Where:

w_s	Particle settling velocity [m/s]
w_0	Particle settling velocity unflocculated, or Stoke [m/s]
$\rho_{sediment}$	Density of grain material
$C_{floc\ min}$	Concentration at which flocculation begins, default set to 0.01 kg/m^3
$C_{floc\ max}$	Concentration at which hindered settling begins, default set to 10 kg/m^3
C_{total}	Total concentration of sediment (sum of concentrations of all fractions)
α :	gradient coefficient, for calibration, default set to 1

5.3 Hindered Settling

In case of fine grained cohesive sediment (<0.006 mm), the size of the particles and thereby the settling velocity will depend on the rate of flocculation.

With low concentrations of suspended sediment, the probability of collision between the cohesive particles is low and the settling velocity will be close to the settling velocity for a single grain. With increasing concentration, collision between particles will occur more frequently and the cohesiveness of the particles will result in formation of flocs. This leads to an increase in average particle/floc size and hereby an increase in settling velocity.

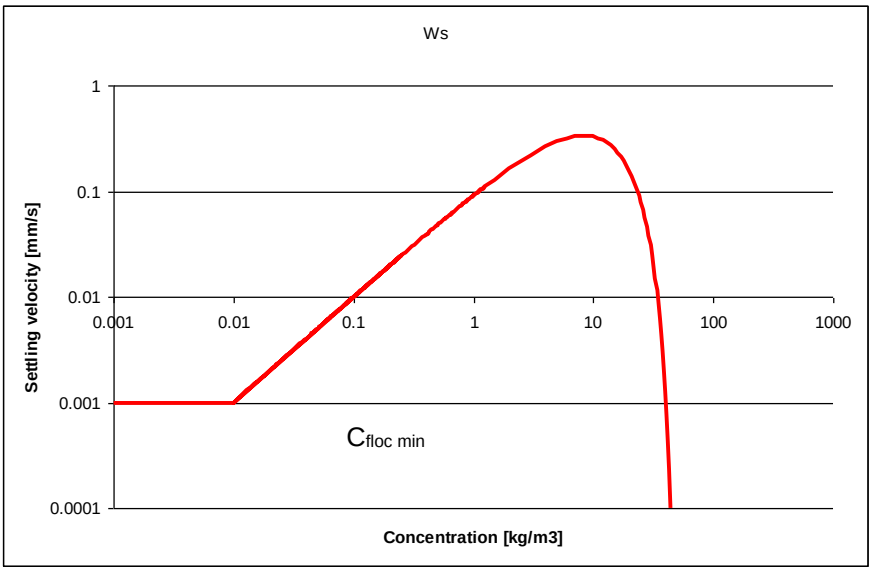

Figure 5.4 The principle of hindered settling where the settling velocity is varying with total concentration

Hindered settling is when the concentration of sediment increases enough to make the flocs influence each other's settling velocity, i.e. the dense concentration prevents the flocs from falling freely. This results in a lower settling velocity. The implemented formulation of hindered settling is based on the formulation of *Richardson and Zaki (1954)*.

$$w_s = w_0 \cdot factor_{floc} \tag{5.6}$$

C_{total} <= $C_{floc\ min}$:

$$factor_{floc} = 1 \tag{5.7}$$

$C_{floc\ min}$ < C_{total}:

$$factor_{floc} = 1 + \alpha \left(\frac{C_{total}}{C_{flocmin}} - 1 \right) \cdot \left(1 - \min \left(1, \frac{C_{total}}{C_{gel}} \right) \right)^5 \tag{5.8}$$

Where:

w_s	Particle settling velocity [m/s]
w_0	Particle settling velocity unflocculated, or Stoke [m/s]
$C_{floc\ min}$	Concentration at which flocculation begins, default set to 0.01 kg/m^3
C_{gel}	Gelling point, default set to 50 kg/m^3
C_{total}	Total concentration of sediment (sum of concentrations of all fractions)
α :	Gradient coefficient, for calibration purpose, default set to 1

5.4 Flocculation Affected by Salinity

In fresh/brackish water, the flocculation processes are reduced, which have an impact on the settling velocity. Due to the smaller floc sizes, the settling velocity will be reduced. This is modelled by multiplying the settling velocity with a corrosion factor, see Equation (5.9).

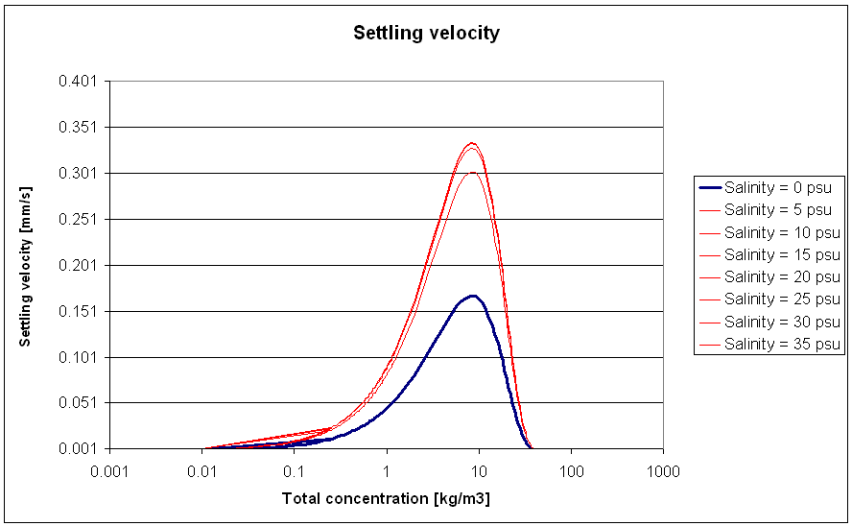

Figure 5.5 Salinity affects the flocculation process. Equation 5.7 used to see effect on settling velocity of salinity at different salinities.

In Figure 5.5, which is based on Equation (5.7) it can be concluded that salinity only plays a significant role on flocculation at salinities below 5 psu. The description of salinity flocculation is based on Krone's experimental research, *Krone 1962*. Whitehouse et al., (1960) studied the effect of varying salinities on flocculation of different clay minerals in the laboratory.

$$w_{s,sali} = w_s\left(1 - c_1 \cdot e^{S \cdot C_2}\right) \tag{5.9}$$

Where:

c_1 and c_2: Calibration parameters.
c_1 and c_2 are not shown in the menu and is default set to
c_1 = 0.5 and c_2 = -0.33

s: Salinity

6 Erosion

Erosion is a process that describes how sediments like mud and sand (with densities larger than water) can get resuspended from the bed into the water column.

The criterion for erosion is that the driving forces exceed the stabilising forces.

The erosion criteria can also be expressed as when the bed shear stress (τ_b) is larger than the critical shear stress for erosion (τ_{ce}).

The erosion is specified individually for each particle class and you have the option to include or exclude the erosion for the individual class.

The flow velocities are normally zero at the bottom and particles in contact with the bed will therefore not move horizontally. If erosion is included and the bed shear stress exceeds the critical shear stress, the particle can perform a random walk through the dispersion term in the vertical direction. In this way the particle can get resuspended into the water column.

6.1 Bed Shear Stress

The bed shear stress τ_b is calculated in the hydrodynamic simulation.
The unit is [N/m^2].

6.2 Critical Bed Shear Stress

The critical bed shear stress is user specified. For mud the critical bed shear stress depends on how consolidated the mud sediments are. For sand the critical bed shear stress is normally estimated based on the work of Shield. Suggestions for estimating the critical bed shear stress are seen in the following.

6.2.1 Mud

Mud type	Density [kg/m^3]	Critical bed shear stress τ_{ce} Typical values [N/m^2]
Mobile fluid mud	180	0.05 – 0.1
Partly consolidated mud	450	0.2 – 0.4
Hard mud	600 +	0.6 – 2.0

6.2.2 Sand

Shields et al. has formulated a way to describe the critical bed shear stress for sand.

$$\tau_{ce} = \theta_{ce} g D(\rho_s - \rho_w) \tag{6.1}$$

Therefore, in order to calculate the critical bed shear stress τ_{ce} the critical Shields' parameter θ_{ce} must be known.

Shields related θ_{ce} to the Reynolds number of the particle to produce a Shields' curve. Brownlie (1981) developed a fit to the Shields' curve. With this relation, the value of θ_{ce} can be computed readily, when the properties of the water and the sediment are given.

$$\theta_{ce} = 0.22 {R_p}^{-0.6} + 0.06 e^{-17.73 {R_p}^{-0.6}} \tag{6.2}$$

$$R_p = \frac{\sqrt{RgD^3}}{\nu} \tag{6.3}$$

$$R = \frac{\rho_s - \rho_w}{\rho_w} \tag{6.4}$$

Where:

τ_{ce}	Critical shear stress
θ_{ce}	Critical Shields' parameter
g	Gravity
D	Diameter of particle
ρ_s	Density of sand
ρ_w	Density of water
ν	Kinematic viscosity

6.3 Resuspension

This process brings particles from the bed shear layer into suspension in the turbulent water column.

As a consequence of the 2 processes, settling and vertical dispersion, a particle can only be brought into suspension if the settling velocity w_s is smaller than the near wall vertical velocity fluctuations from dispersion.

For coarse sediment, this restriction cannot be fulfilled even for large vertical turbulent dispersion near the bed wall. Instead the sediment particles, which have eroded, will fall back to the bed and be transported as bed load, where the particles seem to jump along the bed, switching between erosion and settling. This transport is also called sheet flow.

7 Numerical Solution

7.1 Lagrangian Discrete Parcels Method

In the Particle Tracking Module a Lagrangian discrete-parcel method is used. With this method concentrations or matter in the system are viewed as a large ensemble of small parcels or particles with a specific mass and coordinates for each particle. The movement of each particle and the change in mass is followed and recorded as functions of time independently of reference grid system.

The reference grid system, however, is used when reading the forcings such as the drift velocity for each particle when updating the movement of each particle. From the coordinates of the particle, the drift velocity at the particles position in the reference grid system is found.

After each time step the parcels are summarized in each cell of the reference grid system, and a derived concentration field is calculated using the reference grid system as discretization in space.

$$C_k = \frac{\sum_{i=1}^{N_k} M_i}{V_k} \tag{7.1}$$

Where:

C_k	Concentration in cell k of the reference grid system
k	ID number of cell in reference grid system
M_i	Mass of particle i
N_k	Number of particles within cell k

Thus, the output of the Particle Tracking Module is a list of particles with positions and masses (XML format). From the particle list, the user can also get a derived concentration field.

This Lagrangian discrete parcel method scheme is numerically stable. So the time step of the particle tracking simulation should not be chosen to consider stability, but instead to consider if the phenomenon in question is resolved in time.

7.2 Euler Scheme

The applied random walk method is a simple numerical solution to the Langevin equation. The stochastic differential equation is solved with an explicit Euler scheme:

$$\Delta x = x_n - x_{n-1} = A\left(x_{n-1}, t_{n-1}\right) \cdot \Delta t + \sigma_L \cdot N(0,1) \tag{7.2}$$

Where:

$N(0,1)$	Standard normal distribution ($\mu = 0, \sigma^2 = 1$)
σ_L	Standard deviation of turbulent dispersion $\sigma_L = \sqrt{2 \cdot \Delta t \cdot D_L}$
D	Dispersion coefficient

7.3 The Water Surface Boundary

The forces on a particle (normally hydrodynamic upwelling or buoyancy processes) can drive it to break through the water surface. In the Particle Tracking Module the vertical movement will stop at the water surface, while the horizontal movement of the particle is not manipulated, see Figure 7.1.

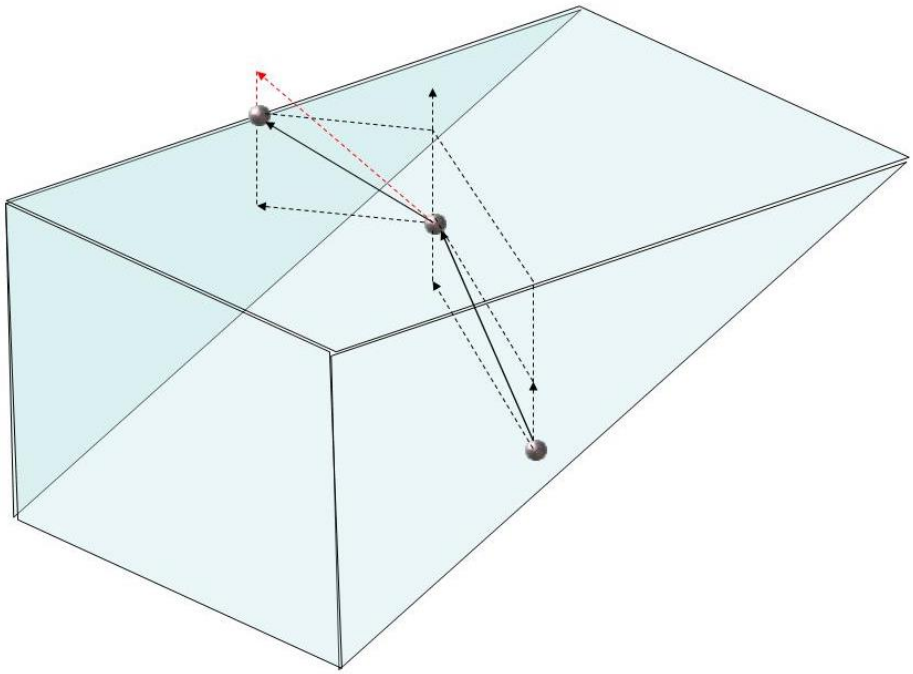

Figure 7.1 The vertical movement vector is cut when a particle reaches the water surface

7.4 The Bed Boundary

If the drift forces of a particle or settling drives it through the bed boundary, it will be stopped at the bed. At this position it will perform a random walk for the diffusion process at the next time step under the condition that the bed shear stress is higher than the critical bed shear stress. The specific random walk for a particle at a given position will be tested: will the random walk pass through the bed layer? If so, a new random walk will be calculated until the movement caused by diffusion will move to somewhere in the water column. The idea is that the probability of moving a given particle to a more shallow area is reduced, so that for instance a closed system with equal concentrations in both shallow and deep zones will remain with equal concentrations.

7.5 The Particle at Dry Point Situation

Once a particle is at a dry position, it will not move until the grid cell is flooded again. Decay can still take place however.

Derived volume concentrations of particles at dry positions do not have a physical meaning, and the user has the option when looking at concentration output of not viewing the “strange” high concentrations at dry grid cells.

Sometimes the particles at dry positions are still important, and in that case it recommended to use the overlay functionality, where the positions of the particles can be viewed on the concentration field including the dry particles, see overlay functionality in Figure 7.2

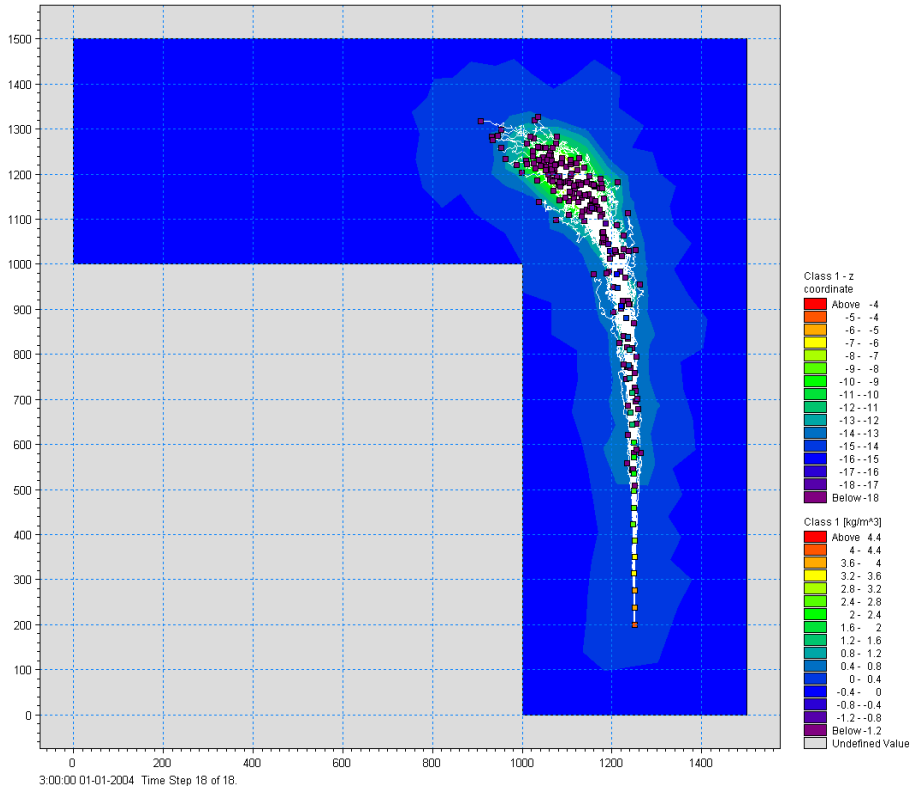

Figure 7.2 It is possible to view the actual particle positions through an overlay functionality when looking at derived concentration fields

7.6 The “Towards Land” Situation

The particle tracks are not allowed to cross land-boundaries. By choosing a relative high time step it is possible to move a particle further than to a neighbour cell. It is therefore not enough to test if the new position is in a valid cell. Instead the particle path to the new destination cell of the particle has to be found, and all the cell borders along the path have to be tested if they are valid to pass through.

If a path goes through a cell border that is land, the particle will not pass through and the path will be projected onto the land border line, see Figure 7.3.

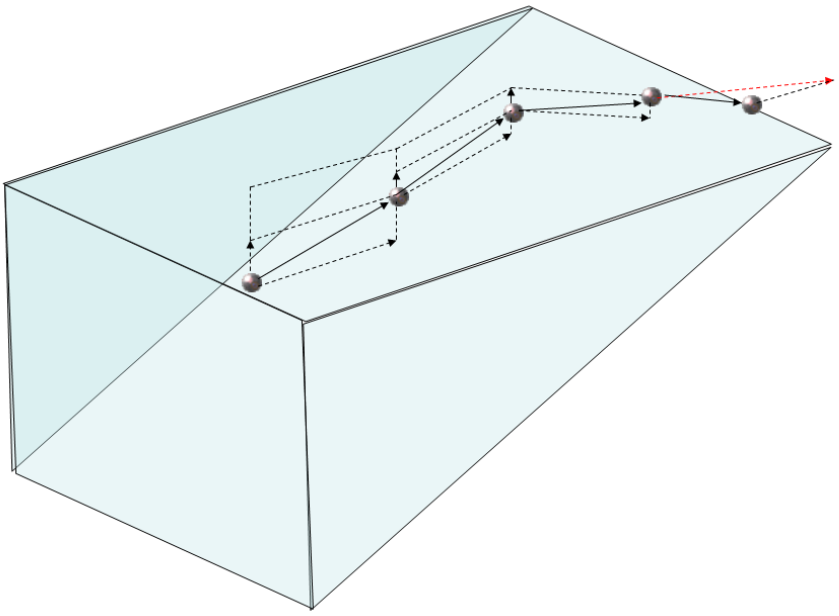

Figure 7.3 The horizontal movement path cannot pass through land borders and instead the path is projected onto the border line

8 References

/1/ Kloeden, (1992): “Numerical Solution of stochastic differential equations”, Springer Verlag Berlin 1992, ISBN 3-540-54062-8.

/2/ Gardiner, C.W., (1983): “Handbook of stochastic Methods for Physics, Chemistry and the Natural Sciences”, Springer Verlag Berlin 1983, ISBN 3-540-15607-0.

/3/ Fischer, H.B., List, E.J., Koh, R., Imberger, J., Brooks, N., (1979): “Mixing in Inland and Coastal Waters”, Academic Press, ISBN 0-12-258150-4.

/4/ Krone, R.B., (1962): “Flume Studies of the Transport of Sediment in Estuarial Processes”, Hydraulic Engineering Laboratory and Sanitary Engineering Research Laboratory, Univ. of California, Berkely, California, Final Report.

/5/ Richardson, J.F., Zaki, W.N, (1954): “Sedimentation and fluidisation: part 1”, Trans. Inst. Chem. Eng. 32, 35– 53.

/6/ Pond, S. Pickard G., (1983): “Introductory Dynamical Oceanography”, Pergamon Press, ISBN 0-08-028728-X.

/7/ Al-Rabeh, A.H., (1994): “Estimating surface oil spill transport due to wind in the Arabian Gulf”, Ocean Engng, Vol. 21 No. 5, pp 461-465.

/8/ Deigaard, R. and E.A. Hansen, (1994): “Simulation of Turbulent Diffusion of Suspended Sediment by a Random Walk Model”, Prog. Rep 75, Institute of Hydrodynamics and hydraulic Engineering, Technical University of Denmark.

/9/ Whitehouse, U.G., Jeffrey, L.M., Debbrecht, J.D., (1960): “Differential settling tendencies of clay minerals in saline waters. In: Swineford (Ed) Clays and clay minerals”, Proceedings 7th National Conference, Pergamon Press, p 1-79.

/10/ Brownlie, W. R. (1981). Prediction of flow depth and sediment discharge in open channels. Report No. KH-R-43A, California Institute of Technology, W. M. Keck Laboratory, Pasedena, CA, 232 pp.

APPENDICES

APPENDIX A

Physical Properties of Water at Different Temperatures

A Kinematic Viscosity

Physical Properties of Water at Atmospheric Pressure								
Temperature		Density[2]	Specific[2] Weight	Dynamic[3] Viscosity	Kinematic[4] Viscosity	Vapour Pressure	Surface[1] Tension	Bulk Modulus
Centigrade	Fahrenheit	Kg/m^3	N/m^3	$N\text{-}s/m^2$	M^2/s	N/m^2abs.	N/m	GN/m^2
0°	32°	1,000	9,810	$1.79x10^{3}$	$1.79x10^{5}$	611	0.0756	1.99
5°	41°	1,000	9,810	$1.51x10^{-3}$	$1.51x10^{-6}$	872	0.0749	2.05
10°	50°	1,000	9,810	$1.31x10^{-3}$	$1.31x10^{-6}$	1,230	0.0742	2.11
15°	59°	999	9,800	$1.14x10^{-3}$	$1.14x10^{-6}$	1,700	0.0735	2.16
20°	68°	998	9,790	$1.00x10^{-3}$	$1.00x10^{-6}$	2,340	0.0728	2.20
25°	77°	997	9,781	$8.91x10^{-4}$	$8.94x10^{-7}$	3,170	0.0720	2.23
30°	86°	996	9,771	$7.97x10^{-4}$	$8.00x10^{-7}$	4,250	0.0712	2.25
35°	95°	994	9,751	$7.20x10^{-4}$	$7.24x10^{-7}$	5,630	0.0704	2.27
40°	104°	992	9,732	$6.53x10^{-4}$	$6.58x10^{-7}$	7,380	0.0696	2.28
50°	122°	988	9,693	$5.47x10^{-4}$	$5.53x10^{-7}$	12,300	0.0679	
60°	140°	983	9.643	$4.66x10^{-4}$	$4.74x10^{-7}$	20,000	0.0662	
70°	158°	978	9.594	$4.04x10^{-4}$	$4.13x10^{-7}$	31,200	0.0644	
80°	176°	972	9,535	$3.54x10^{-4}$	$3.64x10^{-7}$	47,400	0.0626	
90°	194°	965	9,467	$3.15x10^{-4}$	$3.26x10^{-7}$	70,100	0.0607	
100°	212°	958	9,398	$2.82x10^{-4}$	$2.94x10^{-7}$	101,300	0.0589	

[1]Surface tension of water in contact with air
[2]Typical values for sea water are approximately 3 percent higher
[3]Typical values for sea water are approximately 7 percent higher
[4]Typical values for sea water area approximately 4 percent higher