MIKE
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Simple Particle Assessment

MIKE ECO Lab Template

Scientific Description

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1 Introduction

The Simple Particle Assessment (SPA) model template can be used to simulate the fate of a spilled substance subject to decay and evaporation while at the water surface. The movement of the spilled substance is simulated using a Lagrangian particle drift model, based on the advanced possibilities of the DHI Particle Tracking/Oil Spill model core. The decay/ evaporation of the substance is the combination of a simple 1^{st} order background decay process and a complex, age and wind speed dependent surface decay process.

The template can be applied to simulate the spill of chemical substances if the weathering processes are not known in detail but an evaporation/decay information is available e.g. from simple laboratory data/ experiments.

2 Description of the Template

The SPA template defines a passive dispersed particle class with 4 state variables (*Mass*, *RiseVelocity*, *InWater* and *SurfaceTime*) of which two represent internal states (*InWater*, *SurfaceTime*) that cannot be controlled by the user. Another one, *RiseVelocity*, represents the vertical particle speed and is a conservative, non-changing particle property. The rising velocity has been implemented as state variable to allow specifying individual, inter-particle variations in the rising velocity when particles are released. The *Mass* represents the load of the chemical substance per simulated particle.

2.1 State Variables

The following chapter gives a short description for each available state variable and lists the differential equation. Details of the decay model can be found in a later chapter.

2.1.1 Mass

The mass state variable represents the per particle load (instantaneous mass in kg) of the spilled substance. The decay of this mass is dependent on two possible decays process. One is a general, position independent 1st order background decay process. If applied, this decay process is active independent of the particles position in the water column. Contrary, the “SurfaceDecay” process is only active if the particle is on the water surface. Dependent on the total (surface-) age of the particle, this 1st order decay is split into two regimes (i.e. for ‘young’ and ‘old’ spilled particles, mimicking the change of the composition and thus evaporation rate of a spilled substance with time). In each of the two age regimes 4 different, wind depended decay rates can be specified. The applied rate is linearly interpolated between the nearest specifications based on the wind speed an individual particle experiences.

Both decay process are temperature corrected. For details see the decay description below.

$$\frac{d\mathrm{Mass}}{\mathrm{dt}} = -\mathrm{SurfaceDecay} - \mathrm{BackgroundDecay}$$

2.1.2 RiseVelocity

The rising/ vertical velocity of a particle is defined by this state variable. The numeric value is constant during time but may be specified individually for each released particle using the various source options (uniform or from a specified distribution, etc.).

$$\frac{d\mathrm{RiseVelocity}}{\mathrm{dt}} = 0$$

2.1.3 InWater

This state variable represents an internal state/property. In should be initialised by the numeric value “1” when specifying a source definition. A numeric value of “1” refers to a particle in the water phase. Beached or stranded particles will have a numerical value 0. Released particles should always be releases with a numeric value of “1”.

$$\frac{d\mathrm{InWater}}{\mathrm{dt}} = -\mathrm{ChangeImmersedState}$$

2.1.4 SurfaceTime

This variable counts the time (in [sec]) a particle is located on the water surface. It is not necessary identical to the general particle age. It is used to trigger the change of the age based surface decay regime. New released particles should have a numeric value of “0”.

$$\frac{d\mathrm{SurfaceTime}}{\mathrm{dt}} = \mathrm{UpdateSurfaceTime}$$

2.2 Particle Decay

The general background decay is independent on the surface decay, i.e. it is applied independent on the particles position or wind conditions. The surface decay process is just applied if the particle is considered to be at the water surface (controlled by a user specified distance from the surface). It is modelled as a 2-regime process, i.e. there is a general differentiation between “young” and “old” particles. For each regime 4 different decay rates, differentiated by wind speeds, have to be given. Between the different wind speeds the decay rate is linearly interpolated. If a particle is stranded/ beached the surface decay rate can be reduced/modified using an “on-shore” factor.

2.2.1 Temperature dependency

The decay process are temperature compensated, i.e. depended on the ambient temperature. The temperature dependency is modelled as a simple (exponential) Arrhenius dependency with a user specified temperature coefficient and reference temperature. If no temperature dependency is required, the temperature coefficient should be “1.0”.

$$\mathrm{ftemp} = \mathrm{pow}\left(\mathrm{theta}, (\mathrm{Temperature} - \mathrm{RefT})\right)$$

The following table lists selected, relative changes of the rate per 10°C temperature increase and the according values for the temperature coefficient:

Rate change per 10°C increase	Temperature coefficient
0.50	0.933
0.75	0.972
1.00	1.000
1.25	1.023
1.50	1.041
1.75	1.058
2.00	1.072
2.25	1.084
2.50	1.096
2.75	1.106
3.00	1.116
3.25	1.125
3.50	1.133
3.75	1.141
4.00	1.149

Example:
To double the reaction rate (relative change=2.0) if the temperature raises about 10°C you have to select a temperature coefficient of theta=1.072.

2.2.2 Process details

In the following chapter details/equations for the decay process are listed.

$$\mathrm{BackgroundDecay} = k\_bkg * \mathrm{ftemp} * \mathrm{Mass}$$

$$\mathrm{SurfaceDecay} = \text{IF}([\text{BELOW\_SURFACE}] \le \mathrm{minSurfDist}) \begin{cases} \text{THEN} & k * \mathrm{ftemp} * \mathrm{kshore} * \mathrm{Mass} \\ \text{ELSE} & 0 \end{cases}$$

Reduction factor for stranded/beached particles:

$$\mathrm{kshore} = \text{IF}(\mathrm{InWater} > 0.0) \begin{cases} \text{THEN} & 1.0 \\ \text{ELSE} & \mathrm{ShoreDecayFactor} \end{cases}$$

Computation of the surface decay rate:

Linear interpolation between the lower and upper rates for the applied wind regime:

$$k = (\mathrm{kl} + (\mathrm{ku} - \mathrm{kl}) * \mathrm{fwspd})$$

Wind speed factor:

$$\mathrm{fwspd} = \text{IF}(\mathrm{wspdl} < \mathrm{wspdu}) \begin{cases} \text{THEN} & \dfrac{(\mathrm{wspd} - \mathrm{wspdl})}{(\mathrm{wspdu} - \mathrm{wspdl})} \\ \text{ELSE} & 0 \end{cases}$$

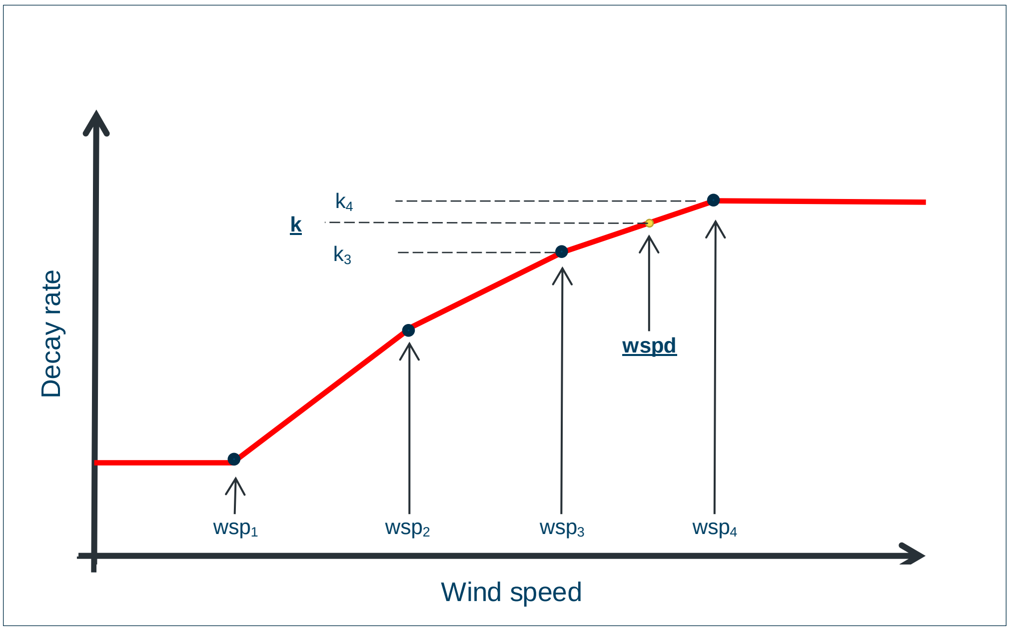

Figure 1 Scheme of the surface decay rate calculation. The wind regime is defined by four wind speeds wsp_1-wsp_4. As example, if the wind speed "***wspd***" is between ***wsp_3*** and ***wsp_4*** the applied decay rate ***k*** is linear interpolated between the upper rate ***k_4*** and the lower rate ***k_3***. Above ***wsp_4*** and below ***wsp_1*** the rate is constant

2.3 Stranding: the Adsorption / Reflection of Particles

The absorbing/reflecting behaviour of land boundaries for particles being washed on shore (stranding) can be controlled by the forcing "BeackLockProbability". This forcing reflects the probability of a particle being absorbed (locked in place) when a stranding occurs. A numeric value of "0.0" disables any absorbing on land boundaries whereas a numeric value of "1.0" corresponds to a 100% chance of absorbing/locking a particle.

Please note that the probability refers to each land contact/stranding event; it does not refer to a time based probability (i.e. probability per time).

The value for "BeackLockProbability" can be specified either globally for the entire model domain or based on a detailed (time varying) 2D map as a dfs2/dfsu file.

2.4 Drift Blocking / Booms

The SPA model supports a simplified blocking model of the particle movement due to obstacles like booms or vegetation etc. The implementation is based on a simplified approach where the user has to specify the chance of a particle being blocked or not. This chance has to be given on a "per time step" base and is applied to all particles within a grid element. This means that you can only control this feature at the grid resolution, sup-grid details are not possible.

The value for "BoomLockProbability" can be specified either globally for the entire model domain or based on a detailed (even time varying) 2D map as dfs2/dfsu file. A numeric value of 0.0 represents no blocking whereas a value of 1.0 is a total movement block (i.e. particles in a grid element with this value will not move).

3 Template Variable Overview

The following chapter lists all defined variables of the SPA model and gives a short description. Variables without need for user interaction are greyed.

3.1 General Constants

Variable	Value*	Description
timestep	Built-in	Model timestep [in sec]

3.2 Forcings

Variable	Value*	Description
hspd	Built-in	Horisontal current speed [m/s]
hdir	Built-in	Horizontal current direction [m/s]
vspd	Built-in	Vertical current speed [m/s]
wspd	Built-in	Wind speed [m/s]
BeackLockProbability	1	Area map with probability of a particle getting absorbed when beached
BoomLockProbability	0	Area map with probability of a particle to not move
Temperature	Built-in	Ambient temperature [°C]

*) Built-in variables are supplied by the hydrodynamic engine automatically. Dependent on the hydrodynamic setup vertical current speed, wind speed and temperature may have to be specified by the user.

3.3 Particle State Variables

Variable	Value*	Description
Mass	10.0	Particle mass/load [kg]
RiseVelocity	0.0	Particle rise velocity [m/s]
InWater	1.0	Indicator if the particle is in the water phase (1) or not (0)
SurfaceTime	0	Time on the surface [sec]

*) The values for ***Mass*** and ***RiseVelocity*** should be defined by the user for the specific project. ***InWater*** and ***SurfaceTime*** should always use the specified default values.

3.4 Particle Class Constants

Variable	Value*	Description
minSurfDist	0.05	Max distance below surface to trigger surface process [m]
ChangeAge	43200	Surface time to change from decay rates a to b [s]
wspd1	1	Wind speed 1 [m/s]
wspd2	2	Wind speed 2 [m/s]
wspd3	3	Wind speed 3 [m/s]
wspd4	4	Wind speed 4 [m/s]
k_1a	1	Decay rate for wind speed 1 and time < change age [/d]
k_2a	2	Decay rate for wind speed 2 and time < change age /d]
k_3a	3	Decay rate for wind speed 3 and time < change age [/d]
k_4a	4	Decay rate for wind speed 4 and time < change age [/d]
k_1b	0.1	Decay rate for wind speed 1 and time >= change age [/d]
k_2b	0.2	Decay rate for wind speed 2 and time >= change age [/d]
k_3b	0.3	Decay rate for wind speed 3 and time >= change age [/d]
k_4b	0.4	Decay rate for wind speed 4 and time >= change age [/d]
k_bkg	0.0	Background decay rate applied independent on particle position
ShoreDecayFactor	1.0	Factor to reduce decay rate once the particle has stranded [0.0-1.0]
RefT	20°C	Reference temperature [°C] for decay rate
theta	1.0	Decay rate temperature dependency

*) The given default values are exemplary and need to be adjusted by the user

3.5 Particle Expressions

Variable	Description	Output
ActSurfaceTime	Current surface time value	-
UpdateSurfaceTime	Update surface time state variable	-
NotBoomLocked	Set to zero to lock a particle at a boom	-
LockAtBeach	Trigger, bmes 1 if particle should be locked on shore	-
AllowMoving	Check if not beached and not boom locked	-
ChangeImmersedState	Change immersed state when particle beaches	-
kua	Upper decay rate for surface time less change age	-
kub	Upper decay rate for surface time >= change age	-
ku	Used decay rate, upper range	-
kla	Lower decay rate for surface time less change age	-
klb	Lower decay rate for surface time >= change age	-
kl	Used decay rate, lower range	-
wspdu	Wind speed, upper range	-
wspdl	Wind speed, lower range	-
fwspd	Wind speed factor	-
k	Used surface decay rate	yes
kshore	Factor to reduce the decay rate once the particle has stranded	-
ftemp	Temperature dependency function	-
SurfaceDecay	Mass decay process on the surface	yes
BackgroundDecay	BackgroundDecay, independent on particle position	yes
DecayPerTimestep	Decay per timestep	yes
setv	Vertical particle speed	-
StrandedMass	Mass stranded on shore	yes
SurfaceMass	Mass on water surface and not stranded	yes
SuspendedMass	Mass suspended below water surface and not stranded	yes

The value of particle expressions with output status can be written as output, either as a (concentration) area/volume files for all particles in a grid element or as individual particle value/item in the particle XML track output. Expressions without output status are internal computational expressions and not visible.