Description of marine dispersion model implemented in ESTE

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The model for calculation dispersion modelling in marine environment implemented in ESTE software tool takes into account three phases: dissolved phase, suspended sediment and bottom (seabed) sediment. The considered interactions between these phases in our approach are:

a) advective transport,
b) diffusion,
c) radioactive decay,
d) burial process on bottom sediment,
e) desorption and adsorption processes,
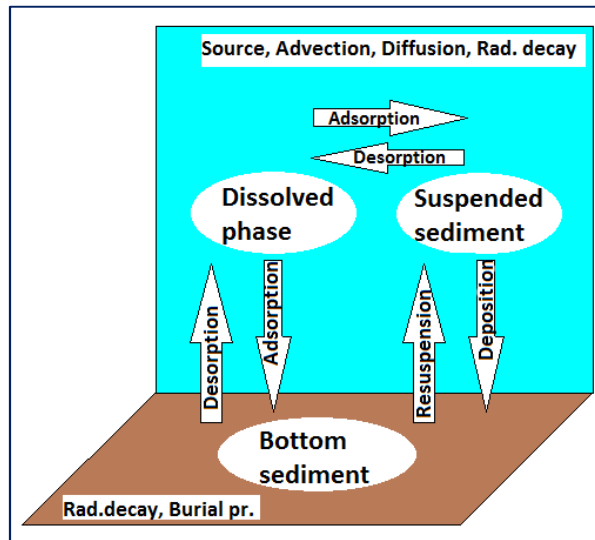f) resuspension and deposition.

Figure: Schematic view of considered interactions between the three phases of marine environment.

The basic equation for the activity concentration in dissolved phase is as follows,

$$\frac{\partial C_{dp}}{\partial t} + \frac{\partial(uC_{dp})}{\partial x} + \frac{\partial(vC_{dp})}{\partial y} + \frac{\partial(wC_{dp})}{\partial z} - \frac{\partial}{\partial x}\left(K_h \frac{\partial C_{dp}}{\partial x}\right) - \frac{\partial}{\partial y}\left(K_h \frac{\partial C_{dp}}{\partial y}\right) - \frac{\partial}{\partial z}\left(K_v \frac{\partial C_{dp}}{\partial z}\right) =$$

$$= -k_{1m}C_{dp} + k_{-1}mC_{ss} - \lambda C_{dp} + S_{dp}, \tag{1}$$

where C_{dp} is the concentration in the dissolved phase, C_{ss} is the activity concentration of the suspended sediment. The terms on the left-hand side represent the advection and diffusion processes, with u, v and w being the components of current velocity. The terms on the right-hand side represent: the first term corresponds to adsorption to suspended sediment, the second term corresponds to desorption from the suspended sediment (m is the concentration of suspended sediment in water), the third term represents

radioactive decay (λ is the decay constant), and the term S_{dp} is the source term. k_{1m} and k_{-1} are kinetic transfer coefficients, related to each other through relation $k_{1m} = k_{-1}mK_d$. Here K_d is sediment distribution coefficient (can be found e.g. in [1]).

The basic equation for the activity concentration in suspended sediment C_{ss} is,

$$\frac{\partial C_{ss}m}{\partial t} + \frac{\partial(uC_{ss}m)}{\partial x} + \frac{\partial(vC_{ss}m)}{\partial y} + \frac{\partial(wC_{ss}m)}{\partial z} - \frac{\partial}{\partial x}\left(K_h \frac{\partial C_{ss}m}{\partial x}\right) - \frac{\partial}{\partial y}\left(K_h \frac{\partial C_{ss}m}{\partial y}\right) - \frac{\partial}{\partial z}\left(K_v \frac{\partial C_{ss}m}{\partial z}\right) =$$

$$= k_{1m}C_{dp} - k_{-1}mC_{ss} - \lambda mC_{ss} + S_{ss}, \tag{2}$$

where the terms on the left-hand side again represent the advection and diffusion processes. The terms on the right-hand side are: the first term corresponds to adsorption from dissolved phase, the second term corresponds to desorption to dissolved phase, the third term represents radioactive decay, and the last term is a possible source term.

In both equations (1) and (2), additional terms occur when including the interactions with bottom sediments. Such interactions include: a) deposition and resuspension for the suspended sediment, and b) desorption from seabed sediment and adsorption from dissolved phase in case of the dissolved phase.

Advection and diffusion processes are solved by lagrangian particle model. The movement of each particle is described by equations:

$$x_{t+\Delta t} = x_t + u.\Delta t + dx_{dif}, \tag{3a}$$

$$y_{t+\Delta t} = y_t + v.\Delta t + dy_{dif}, \tag{3b}$$

$$z_{t+\Delta t} = z_t + w.\Delta t + dz_{dif}, \tag{3c}$$

where $\vec{x} = (x, y, z)$ specifies the position of the particle (at the times t and $t + \Delta t$), Δt is the time step, $\vec{v} = (u, v, w)$ is the velocity vector of the current field for the given time t and position $\vec{x}$. $\overrightarrow{dx_{dif}} = (x_{dif}, y_{dif}, z_{dif})$ represent the random walk terms describing the diffusion process. They are based on the model [2], and satisfy the relations

$$dx_{dif} = \sqrt{12K_h\Delta t}.r_0.\cos(2\pi r_1), \tag{4a}$$

$$dy_{dif} = \sqrt{12K_h\Delta t}.r_0.\sin(2\pi r_1), \tag{4b}$$

$$dz_{dif} = \sqrt{6K_v\Delta t}.r_2, \tag{4c}$$

where r_0 and r_1 are random numbers between 0 and 1, r_2 is a random number between -1 and 1. K_h is the horizontal diffusion coefficient and K_v is the vertical diffusion coefficient. K_h is evaluated using the Smagorinsky formula [3]:

$$K_h = C\Delta x\Delta y\sqrt{\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2}, \tag{5}$$

where C is a constant equal to 0.05, Δx and Δy represent the scale of motion.

In all three phases, **radioactive decay** is taken into account. The **burial process** is considered as a decay process, (characterized by λ_{burial}), causing a decrease of activity in the bottom sediment. Its value is estimated as

$$\lambda_{burial} = \frac{SR}{\rho L_{bs}}, \tag{6}$$

where SR is sedimentation rate, ρ is bulk density of bottom sediment, and L_{bs} is depth of the upper sediment layer.

The program involves a simple **model for biological uptake** which enables to evaluate activity concentration in marine animals (e.g. in fish). The evaluation is based on the determined activity concentration in the dissolved phase (mean value in a certain time period) and concentration factors for biological material. The concentration in marine organisms c_{mo} (concentration per unit mass of organism, in unit of Bq/kg) is given as

$$c_{mo} = CF.c_{sw}. \tag{7}$$

Here CF is concentration factor (in unit of L/kg, given in [1]), and c_{sw} is concentration in seawater (dissolved phase, in unit of Bq/L). The factors CF are determined for fishes, mollusks, crustaceans, planktons and algae, and for a large number of elements.

Literature:

[1] - IAEA Technical Reports Series No. 422 (2004) - TRS422: "Sediment Distribution Coefficients and Concentration Factors for Biota in the Marine Environment".

[2] – Perianez R. and Elliott A.J., A particle-tracking method for simulating the dispersion of non-conservative radionuclides in coastal waters, J. Environ. Radioactivity 58 (2002) 13–33.

[3] – Smagorinsky J., General circulation experiments with primitive equations. 1. The basic experiment. Monthly Weather Review 91 (1963): 99–164.