Heavy Metal

MIKE ECO Lab Template

Scientific Description

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1 Introduction

MIKE ECO Lab is a numerical lab for Ecological Modelling. It is a generic and open tool for customising aquatic ecosystem models to describe for instance water quality. DHI's expertise and know how concerning ecological modelling has been collected in predefined ecosystem descriptions (MIKE ECO Lab templates) to be loaded and used in MIKE ECO Lab. So the MIKE ECO Lab templates describe physical, chemical and biological processes related to environmental problems and water pollution. The following is a description of the DHI supported Heavy Metal template.
It is a revision of the former ME template.

The heavy metal template is used in investigations of heavy metal spreading and potential accumulation in sediment. The heavy metal template can be applied in environmental impact assessments concerning:

- spreading of heavy metals from urban and/or industrial discharges

- leakages of heavy metals from disposal sites (fly ash disposals, cinders disposals, metal or chemical land dump sites etc.)

- spreading of metals from dumping/waste disposal activities at sea

- accumulation of metals in sediment and potentially in biota

- release or leakage of metals formerly dumped or accumulated in the sediment resulting in further spreading and 'dilution' of the sediments.

- dredging and other operations disturbing the sediment leading to a re-introduction of the sorbed metals into the water.

The heavy metal template describes the adsorption/desorption of metals to suspended matter, the sedimentation of sorbed metals to the seabed as well as resuspension of settled metal. It also includes the exchange of metal between the particulates of the bed sediment and the interstitial waters of the bed. The diffusive exchange of metal in dissolved form in the water and in the interstitial waters is also described.

A number of derived values are calculated for instance the total concentration of metal in the water and in the bed sediment (the sum of dissolved and adsorbed metal).

The various metals behave very differently. The template is therefore designed as a general model with the relevant processes included and then with a number of metal specific parameters. Once the parameters for a metal have been settled this set-up can be said to be a model for this specific metal.

The model results are the concentrations of dissolved heavy metal, adsorbed metal and of suspended matter in the water (per volume) and the dissolved metal in interstitial waters of the bed sediment, the metal adsorbed to particles in the bed sediment and finally the thickness of the considered sediment layer. In addition to this the above mentioned derived values are stored.

The heavy metal template is integrated with the advection-dispersion module, which describes the physical transport and spreading processes at each grid point covering the area of interest.

2   Theoretical Aspects of Heavy Metal Spreading

Heavy metals in the aquatic environment will be found dissolved in the water or attached to suspended matter. The extent to which a heavy metal is bound to the suspended matter differs from metal to metal and it also depends on the nature of the suspended particles. The adsorption to suspended matter leads to sedimentation of heavy metal, which will often look like a disappearance. It is rather just a transport out of the water column into the sediment. This apparent cleaning of the water is often called "scavenging" (Nyffeler et.al., 1986).

The heavy metals will reappear in the sediment together with the sedimented particles. Heavy metals can remain in the sediment attached to the particles even long time after the pollution has stopped (de Bruijn et.al., 1989).

In the sediment the conditions for adsorption are very different from the water phase conditions, due to differences in particle concentration. The heavy metal concentration in the pore water of the sediment will therefore differ from the water column concentration resulting in diffusive transport between sediment and water. This is one of the mechanisms by which heavy metals are transported from polluted sediment to more clean water. The other mechanism is resuspension of the sediment.

The consequences of discharging heavy metal into the aquatic environment or the mobility of metal from formerly polluted sediment can be predicted by modelling the mechanisms governing the transport of heavy metals. On a molecular level these mechanisms are numerous, but in a macroscopic scale a limited number of overall processes seems to be governing (Honeyman & Santschi, 1988; Anderson et.al., 1987):

1. The adsorption and desorption of metal
2. The sedimentation and resuspension of particulate metal
3. The diffusive transport of dissolved metal at the sediment/ water interface
4. The transport of dissolved and particulate metal in the water column by advection and dispersion.

The Heavy Metal MIKE ECO Lab template itself accounts for the first 3 mentioned overall processes, whereas the advection-dispersion process is calculated in the software product that has MIKE ECO Lab implemented: for instance MIKE 11 or MIKE 21. So the scientific documentation for the advection-dispersion process must be found in the manuals for the used product.

In the Heavy Metal Template a kinetic approach to describe the distribution of heavy metals between water and particles has been chosen for two reasons.

First, the time to reach equilibrium between water and particles has turned out to be in the range 'day to week' when the measuring is based on natural sediment (Honeyman & Santschi, 1988; Nyffeler et.al.,1986). This is contradictory to results of measurements based on artificial sediment composed of a limited number of minerals. Here the adsorption and desorption rates were found to be too fast to have significant influence on the scavenging (DiToro et.al., 1986). As the residence time of particles in the water column of shallow waters usually is within the range mentioned above (day to week), the time to reach equilibrium may be longer than the residence time of the particles. In this case the equilibrium assumption is not valid.

Secondly, the only rational way to account for the diffusive transport of dissolved metals at the sediment/water interface is to use the kinetic approach. Otherwise, several consecutive iteration schemes must be introduced to fulfil the equilibrium constraint and describe the diffusive transport (Chapman, 1982).

The terms "sorption", "adsorption" or "desorption" are here generic terms used to describe the transport of solute from the solution phase to a contiguous solid phase or reverse. In principle an aqueous solute (be it dissolved heavy metal) may react with a preexisting solid phase by three main processes (Honeyman & Santschi, 1988):

• adsorption (attachment at the interface without development of a three-dimensional molecular arrangement)

• absorption (the incorporation of chemical solute into the solid phase)

• surface precipitation

In this model these terms are viewed as one overall process. The rates of the above listed individual processes and the relevance of each of them are not considered.

The sorption of the heavy metals depends on the nature of the particulate matter due to varying mechanisms (from metal to metal) for the sorption.

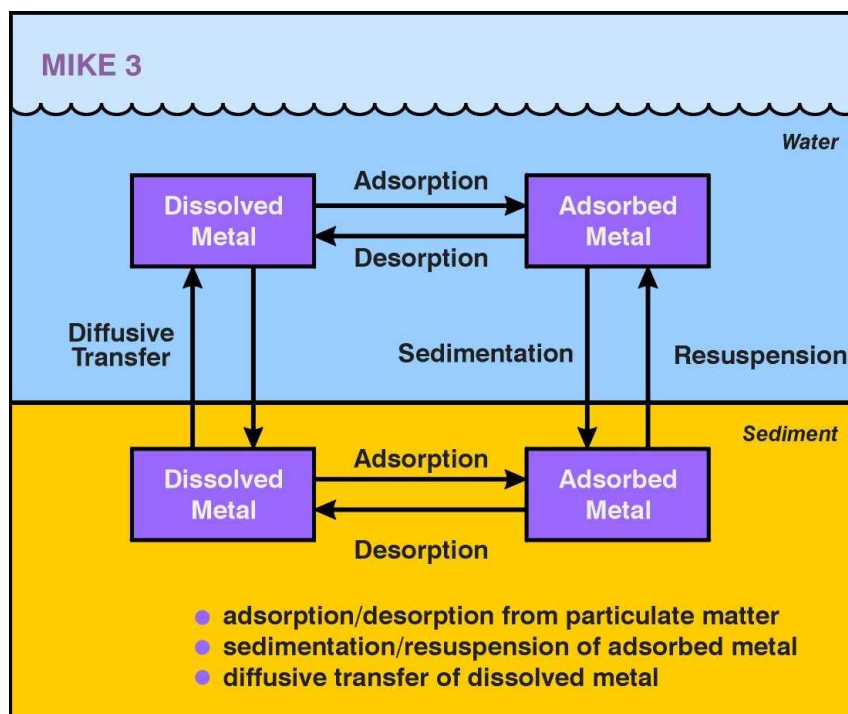The processes of the Heavy Metal MIKE ECO Lab template are schematically summarised in Figure 2.1.

Figure 2.1   Sketch showing the transfer processes included in the Heavy Metal template

Adsorption and desorption are reverse reactions for the transition of metal between solute (Cw, concentration in water, g/m3) and solid (Cs, concentration on solid, g/g) phases:

$$C_w \underset{\leftarrow}{\overset{\rightarrow}{}} C_s \qquad\qquad (2.1)$$

where the forward reaction ($\rightarrow$) is the adsorption and the reverse reaction ($\leftarrow$) is the desorption.

Due to differences in the characteristics of the particulate matter in the water column and the sediment, the adsorption and desorption processes can be different in the sediment and the water column respectively.

The suspended matter and the metal attached to it can settle and be resuspended depending on the hydraulic conditions. This exchange of particles between water and sediment is one way of exchanging heavy metal. The other is the diffusive transport between water and pore water due to concentration differences (Santschi,1988).

The balance for suspended solids in the water phase includes settling, resuspension and production of particles (e.g. detritus (degrading biomass) or micro algae).

The direct exchange of metals between water and pore water is assumed to be a diffusive process, driven by the concentration gradient over a thin stagnant water layer at the water/sediment interface (Jørgensen, 1979; Nyffeler et.al.,1986; Santschi et.al.,1987).

3 Mathematical Formulations

In the following all symbols for state variables distinguish between soluble S and particulate X.

The considered dependent state variables in the model are:

S_{HM} Dissolved heavy metal conc. in the water [gMe/m³ bulk]

X_{HM} Adsorbed heavy metal conc. in the water [gMe/m³ bulk]

X_{SS} Suspended solids conc. in the water [g DW/m³ bulk]

S_{HMS} Dissolved heavy metal conc. in sediment [gMe/m²]

X_{HMS} Adsorbed heavy metal conc. in sediment [gMe/m²]

X_{SED} Mass of sediment [g DW/m²]

The theoretical basis and the assumptions connected with the mathematical formulations of the involved processes for the heavy metals are outlined above. Furthermore, it is necessary to introduce some assumptions concerning the sediment layer.

The part of the sediment layer included in this model is the top 10 centimeters or so, being homogeneous (Nyffeler, 1984). It is assumed that the composition of the sediment concerning porosity and density of particles and pore water is constant in time. The consequences of sedimentation or resuspension are not a change in concentration of particles in the sediment, but a change in sediment layer thickness.

Heavy metal dissolved in the water S_{HM}

$$\frac{dS_{HM}}{dt} = -adsorption + desorption + diffusion \qquad (3.1)$$

$$\frac{dS_{HM}}{dt} = -adss + dess + difv \qquad \text{[gMe/m}^3\text{ bulk/d]}$$

Adsorption
The partitioning coefficient K_d can be described as the relation between heavy metal content in the suspended matter and concentrations in the water phase at steady state.

The heavy metals are mostly bound to the organic part of the suspended matter, therefore the K_d partitioning coefficient is estimated from of the organic carbon partitioning coefficient for the metal in question, and the fraction of organic carbon in the suspended matter:

$$K_d = f_{OC} \cdot K_{OC} \qquad (3.2)$$

Where:
f_{OC} Fraction of organic carbon in the suspended solids (mg/mg).

K_{OC} Organic Carbon Partitioning coefficient [l / kg DW]. K_{OC} is the key parameter in the heavy metal template, and it is different for each heavy metal. It is also dynamic, and depends on temperature, pH,

salinity, and pe. Therefore the user should give K_{OC} values based on measurements at the conditions in the model regarding temperature, pH, salinity, and pe. If these measurements do not exist the K_{OC} is a calibration parameter.

Table 3.1 gives examples of the magnitude of K_d for different heavy metals.

Table 3.1   Partition coefficients K_d for metals between sediment and water, both estimated values and values based on monitoring data. Fraction of organic carbon is 10% and clay content is 25% in the particulate matter

Metal	Log K_d (sed/water) Estimated[1] [l/kg]	Log K_d(sed/water) Monitoring data[2] [l/kg]
Antimony	3.41	
Arsenic	3.82	4.07
Barium	3.00	
Beryllium	2.78	
Cadmium	4.93	4.90
Chromium	5.28	5.15
Cobalt	3.60	
Copper	4.53	4.22
Lead	5.63	5.18
Mercury	5.05	4.56
Molybdenum	2.93	
Nickel	3.72	3.99
Selenium	2.62	
Thalium	3.00	
Tin	6.09	
Vanadium	3.59	
Zinc	4.86	4.82

The adsorption and desorption rates are assumed to be related relative to each other according to the equilibrium partitioning coefficient K_d for the metal in question:

$$K_d = \frac{k_a}{k_w}$$

(3.3)

Where:

k_w Desorption rate in water [d^{-1}]
k_a Adsorption rate [m^3 H$_2$O /g DW / d]

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[1]   Estimated values on the basis of partition coefficients between particulate mattter and water (Stortelder et al, 1989)

[2]   Values based on monitoring; data in freshwater and sediment at 3 different locations in the Netherlands and different time-intervals (Venema, 1996)

K_d	Partitioning coefficient for metal between particulate matter and water [m³ H₂O / g DW]

Therefore it is only necessary to know one of the sorption rates and the partitioning coefficient to estimate the opposite sorption rate. This has been used in the following to exclude the adsorption rate k_a from the equations and replace it by k_w and K_d.

The following assumption has been made: m³ H₂O ≈ m³ bulk

$$adss = k_w \cdot K_d \cdot S_{HM} \cdot X_{SS} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \qquad (3.4)$$

Where:

k_w	Desorption rate in water [d⁻¹]
K_d	Partitioning coefficient for metal between particulate matter and water [m³ H₂O / g DW]
S_{HM}	Dissolved heavy metal conc. in the water water [g Me/m³ bulk] ≈ [g Me/m³ H₂O]
X_{SS}	Suspended solids conc. in the water [g DW/m³ bulk]

Desorption

The adsorbed heavy metals can be desorbed from the adsorbed phase to the dissolved phase in the water column.

$$dess = k_w \cdot X_{HM} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \qquad (3.5)$$

Where:

k_w	Desorption rate in water [d⁻¹]
X_{HM}	Adsorbed heavy metals conc. in the water [g Me/m³ bulk]

Diffusion

According to Fick's law, gradients in concentration fields can cause diffusion. In this template diffusion can take place between dissolved heavy metals in the water column and in the porewater of the sediment.

$$difv = \frac{fbiot \cdot difw \cdot \left(\frac{S_{HMS}}{pors \cdot dzs} - S_{HM}\right)}{(dzwf + dzds) \cdot dz} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \qquad (3.6)$$

Where:

$fbiot$	Factor for diffusion due to bioturbation [dimensionless]
$difw$	Diffusion coefficient in water is estimated from the metals moleweight [m²/d]
S_{HM}	Dissolved heavy metal conc. in the water [g Me/m³ bulk] ≈ [g Me/m³ H₂O]
S_{HMS}	Dissolved heavy metal conc. in sed. porewater [g Me/m²]
$dzwf$	Thickness of water film [m]
$dzds$	Thickness of diffusion layer in sediment [m]
dz	Thickness of actual layer in computational grid [m]

Heavy metal on suspended matter X_{HM}

$$\frac{dX_{HM}}{dt} = adsorption - desorption - sedimentation + resuspension \tag{3.7}$$

$$\frac{dX_{HM}}{dt} = adss - dess - sev + resv \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right]$$

Adsorption
See also description of adsorption for S_{HM}.

$$dess = k_w \cdot X_{HM} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \tag{3.8}$$

Where:
k_w Desorption rate in water [d^{-1}]
K_d Partitioning coefficient for metal between particulate matter and water [m^3 H$_2$O / g DW], see table 1
S_{HM} Dissolved heavy metal conc. in the water [g Me/m^3 bulk] $\approx$ [g Me/m^3 H$_2$O]
X_{SS} Suspended solids conc. in the water [g DW/m^3 bulk]

Desorption
The adsorbed heavy metals can be desorbed from the adsorbed phase to the dissolved phase in the water column.

$$dess = k_w \cdot X_{HM} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \tag{3.9}$$

Where:
k_w Desorption rate in water [d^{-1}]
X_{HM} Adsorbed heavy metals conc. in the water [g Me/m^3 bulk]

The unit of *dess* is g heavy metal per volume bulk.

Sedimentation
The adsorbed heavy metals will be transported with the suspended solid, that normally are affected by a sedimentation process. The sedimentation of suspended solids is described with a settling velocity.

$$sev = \frac{vsm \cdot X_{HM}}{dz} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \tag{3.10}$$

Where:
vsm Settling velocity of SS [m/d]
X_{HM} Adsorbed heavy metals conc. in the water [g Me/m^3 bulk]
dz Thickness of actual layer in computational grid [m]

Resuspension
The adsorbed heavy metals in the sediment can be resuspended if the suspended matter is brought into suspension in the water column. This can occur when the current speed exceeds a critical value.

if $(cspd > ucrit)$:

$$resv = \frac{resrat \cdot \dfrac{X_{HMS}}{X_{SED}}}{dz} \qquad \left[\frac{gMe}{m^3 bulk \cdot d}\right] \qquad (3.11)$$

Where:
cspd	Current Speed adjusted for sediment build up [m/s]
ucrit	Critical current speed for resuspension of SS [m/s]
resrat	Resuspension rate of SS [gDW/m²/day]
X_{HMS}	Adsorbed heavy metals conc. in the sediment [g Me/m²]
X_{SED}	Mass of sediment [g DW/m²]
dz	Thickness of actual layer in computational grid [m]

Suspended matter or solids in the water X_{SS}

$$\frac{dX_{SS}}{dt} = production - sedimentation + resuspension \qquad (3.12)$$

$$\frac{dS_{SS}}{dt} = prss - sessv + ressv \qquad \left[\frac{gDW}{m^3 bulk \cdot d}\right]$$

Production
Suspended matter can be produced in the water column by primary production. The rate of particle production is specified as a fixed coefficient parpro:

$$prss = \frac{parpro}{dz} \qquad \left[\frac{gDW}{m^3 bulk \cdot d}\right] \qquad (3.13)$$

Where:
parpro	Particle production rate [gDW/m²/day]
dz	Thickness of actual layer in computational grid [m]

Sedimentation
The suspended matter is affected by a sedimentation process. The sedimentation of suspended solids is described with a settling velocity.

$$sessv = \frac{vsm \cdot X_{SS}}{dz} \qquad \left[\frac{gDW}{m^3 bulk \cdot d}\right] \qquad (3.14)$$

Where:
vsm	Settling velocity of SS [m/d]
X_{SS}	Suspended solids conc. in the water [g DW/m³ bulk]
dz	Thickness of actual layer in computational grid [m]

Resuspension
The sediments can be resuspended when the current speed exceeds a critical value.

if $(cspd > ucrit)$:

$$ressv = \frac{resrat}{dz} \qquad \left[\frac{gDW}{m^3 bulk \cdot d}\right] \qquad (3.15)$$

Where:
cspd	Current Speed adjusted for sediment build up [m/s]
ucrit	Critical current speed for resuspension of SS
resrat	Resuspension rate of SS [gDW/m²/day]
dz	Thickness of actual layer in computational grid [m]

Dissolved heavy metal in the sediment S_{HMS}

$$\frac{dS_{HMS}}{dt} = \text{- adsorption + desorption – diffusion}$$ (3.16)

$$\frac{dS_{HMS}}{dt} = -adsa + desa - difa \qquad \left[\frac{gMe}{m^2 \cdot d}\right]$$

Adsorption

The adsorption and desorption rates are assumed to be related relative to each other according to the equilibrium partitioning coefficient K_d for the metal in question:

$$K_{ds} = \frac{k_a}{k_s} \qquad \text{[m}^3\text{ H}_2\text{O / g DW]}$$ (3.17)

Where:
k_s	Desorption rate in sediment [d⁻¹]
k_a	Adsorption rate [m³ H₂O /g DW / d]
K_{ds}	Partitioning coefficient for metal between particulate matter and water [m³ H₂O / g DW] , see Table 3.1

Therefore it is only necessary to know one of the sorption rates and the partitioning coefficient to estimate the opposite sorption rate. This has been used in the following to exclude the adsorption rate k_a from the equations and replace it by k_s and $K_{ds.}$

The unit for adsorbed heavy metals in the pore water of the sediment is g heavy metal per volume bulk.

$$adsa = k_s \cdot K_{ds} \cdot S_{HMS} \cdot \frac{X_{SED}}{dzs \cdot por_s} \qquad \left[\frac{gMe}{m^2 \cdot d}\right]$$ (3.18)

Where:
k_s	Desorption rate in sediment [d⁻¹]
K_{ds}	Partitioning coefficient for metal between particulate matter and water [m³ H₂O / g DW] , see Table 3.1
S_{HMS}	Dissolved heavy metal conc. in the sediment [gMe/m²]
dzs	Sediment layer thickness [m]
X_{SED}	Mass of sediment (g DW/m²)
por_s	Porosity of sediment [m³ H₂0 / m³ bulk], assumed constant

Desorption

The adsorbed heavy metals in the sediment can be desorbed from the adsorbed phase to the dissolved phase in the pore water.

$$desa = k_s \cdot X_{HMS} \qquad \left[\frac{gMe}{m^2 \cdot d}\right] \qquad (3.19)$$

Where:

k_s	Desorption rate in sediment [kg / l / d]
X_{HM}	Adsorbed heavy metals conc. in the water [g Me/m³ bulk]

Diffusion

According to Fick's law, gradients in concentration fields can cause diffusion. In this template diffusion can take place between dissolved heavy metals in the water column and in the porewater of the sediment.

$$difa = \frac{fbiot \cdot difw \cdot \left(\dfrac{S_{HMS}}{por_s \cdot dzs} - S_{HM}\right)}{dzwf + dzds} \qquad \left[\frac{gMe}{m^2 \cdot d}\right] \qquad (3.20)$$

Where:

fbiot	Factor for diffusion due to bioturbation [dimensionless]
difw	*D*iffusion coefficient in water is estimated from the metals moleweight [m²/d]
S_{HM}	Dissolved heavy metal conc. in the water [g Me/m³ bulk] ≈ [g Me/m³ H₂O]
S_{HMS}	Dissolved heavy metal conc. in sed. porewater [g Me/m²]
dzwf	Thickness of water film
dzds	Thickness of diffusion layer in sediment
dzs	Sediment layer thickness [m]
por_s	Porosity of sediment [m³ H₂0 / m³ Bulk]

Heavy metal attached to sediment X_{HMS}

$$\frac{dX_{HMS}}{dt} = adsorption - desorption + sedimentation - resuspension \qquad (3.21)$$

$$\frac{dX_{HMS}}{dt} = adsa - desa + sea - resa \qquad \left[\frac{gMe}{m^2 \cdot d}\right]$$

Adsorption

The adsorption and desorption rates are assumed to be related relative to each other according to the equilibrium partitioning coefficient K_d for the metal in question:

$$K_{ds} = \frac{k_a}{k_s} \qquad [\text{m}^3 \text{ H}_2\text{O / g DW}] \qquad (3.22)$$

Where:

k_s	Desorption rate in sediment [d⁻¹]
k_a	Adsorption rate [m³ H₂O /g DW / d]
K_{ds}	Partitioning coefficient for metal between particulate matter and water [m³ H₂O / g DW], see Table 3.1

Therefore it is only necessary to know one of the sorption rates and the partitioning coefficient to estimate the opposite sorption rate. This has been used in the following to exclude the adsorption rate k_a from the equations and replace it by k_s and K_{ds}.

The unit for adsorbed heavy metals in the water column is g heavy metal per volume bulk.

$$adsa = k_s \cdot K_{ds} \cdot S_{HMS} \cdot \frac{X_{SED}}{dzs \cdot por_s} \qquad \left[\frac{gMe}{m^2 \cdot d} \right] \tag{3.23}$$

Where:

k_s	Desorption rate in sediment [d^{-1}]
K_{ds}	Partitioning coefficient for metal between particulate matter and water [m^3 H$_2$O / g DW] , see Table 3.1
S_{HMS}	Dissolved heavy metal conc. in the sediment [gMe/m^2]
dzs	Sediment layer thickness [m]
X_{SED}	Mass of sediment (g DW/m^2)
por_s	Porosity of sediment [m^3 H$_2$0 / m^3 bulk], assumed constant

Desorption
The adsorbed heavy metals in the sediment can be desorbed from the adsorbed phase to the dissolved phase in the pore water.

$$desa = k_s \cdot X_{HMS} \qquad \left[\frac{gMe}{m^2 \cdot d} \right] \tag{3.24}$$

Where:

k_s	Desorption rate in sediment [d^{-1}]
X_{HMS}	Adsorbed Heavy Metals in the sediment [g Me/m^2]

Sedimentation
The suspended matter is affected by a sedimentation process. The sedimentation of suspended solids is described with a settling velocity.

$$sea = vsm \cdot X_{HM} \qquad \left[\frac{gMe}{m^2 \cdot d} \right] \tag{3.25}$$

Where:

vsm	Settling velocity of SS [m/d]
X_{HM}	Adsorbed heavy metal conc. in the water [gXe/m^3 bulk]

Resuspension
The adsorbed heavy metals in the sediment can be resuspended if the suspended matter is brought into suspension in the water column. This can occur when the current speed exceeds a critical value.

$$\text{if } (cspd > ucrit): $$
$$resa = \frac{resrat \cdot X_{XES}}{X_{SED}} \qquad \left[\frac{gMe}{m^2 \cdot d} \right] \tag{3.26}$$

Where:

$cspd$	Current Speed adjusted for sediment build up [m/s]
$ucrit$	Critical current speed for resuspension of SS

resrat	Resuspension rate of SS [gDW/m²/day]
X_{XES}	Adsorbed Xenobiotics in the sediment [g Xe/m²]
X_{SED}	Mass of sediment [g DW/m²]

Mass of sediment X_{SED}

$$\frac{dX_{SED}}{dt} = sedimentation - resuspension \tag{3.27}$$

$$\frac{dX_{SED}}{dt} = sessa - ressa \qquad \left[\frac{gDW}{m^2 \cdot d}\right]$$

Sedimentation
The suspended matter in the water column is affected by a sedimentation process. The sedimentation of suspended solids is described with a settling velocity.

$$sessa = vsm \cdot X_{SS} \qquad \left[\frac{gDW}{m^2 \cdot d}\right] \tag{3.28}$$

Where:

vsm	Settling velocity of SS [m/d]
X_{SS}	Suspended solids conc. in the water [g DW/m³ bulk]

Resuspension
The sediments are resuspended when the current speed exceeds a critical value.

$$\text{if } (cspd > ucrit): \qquad \left[\frac{gDW}{m^2 \cdot d}\right] \tag{3.29}$$
$$ressa = resrat$$

Where:

cspd	Current Speed adjusted for sediment build up [m/s]
ucrit	Critical current speed for resuspension of SS
resrat	Resuspension rate of SS [gDW/m²/day]

4 Data Requirements

- Basic Model Parameters
    - Model grid size and extent
    - Time step and length of simulation
    - Type of output required and its frequency

- Bathymetry and Hydrodynamic Input

- Combined Advection-Dispersion Model
    - Dispersion coefficients

- Initial Conditions
    - Concentration of state variables

- Boundary Conditions
    - Concentration of state variables

- Pollution Sources
    - Discharge magnitudes and concentration of relevant state variables

- Process Rates
    - Size of coefficients governing the process rates. Some of these coefficients can be determined by calibration. Others will be based on literature values or found from actual measurements and laboratory tests.

5 References

/1/ Anderson, Robert F., Peter H. Santschi, Urs P. Nyffeler & Sherry L. Schiff, 1987. "Validating the Use of Radiotracers as Analogs of Stable Metal Behaviour in Enclosed Aquatic Ecosystem Experiments". Can. J. Fish. Aquat. Sci., Vol. 44, pp. 251-259.

/2/ de Bruijn, B., B. de Boer & A.M. Van der Mejden, 1989. "Simulation Model for the Long Term Development of Water and Sediment Quality in Major Dutch Rivers and Lakes". Water Pollution Research Report No. 19, CEC. Proceedings of the COST 641 (Working Party 2) Workshop held in Bilthaven, The Netherlands, 20 - 21 April, 1989.

/3/ Chapman, Bernard M, 1982. "Numerical Simulation of the Transport and Speciation of Nonconservative Chemical Reactants in Rivers". Water Resources Research, Vol. 18, No. 1, pp. 155-167.

/4/ Di Toro, Dominic M., John D. Mahony, Paul R. Kirchgraber, Ann L. O'Byrne, Louis R. Pasquale & Dora C. Piccirilli, 1986. "Effects of Nonreversibility, Particle Concentration, and Ionic Strength on Heavy Metal Sorption". Environ. Sci. Technol., Vol. 20, No. 1., pp. 55-61.

/5/ Honeyman, Bruce D. and Peter H. Santschi, 1988. "Metals in aquatic systems". Environ. Sci. Technol. Vol 22, No. 8, pp. 862-871.

/6/ Jannasch, Hans W., Bruce D. Honeyman, Laurie S. Balistrieri & James W. Murray, 1988. "Kinetics of trace element uptake by marine particles". Geochim. Cosmochim. Acta, Vol. 52, pp. 567-577.

/7/ Jørgensen, Sven Erik, 1979. "Modelling the Distribution and Effect of Heavy Metals in an Aquatic Ecosystem". Ecological Modelling, 6, pp. 199-222.

/8/ Nyffeler, Urs P., Peter H. Santschi & Yuan-Hui Li, 1986. "The relevance of scavenging kinetics to modelling of sediment-water interactions in natural waters". Limnol. Oceanogr., 31(2), pp. 277-292.

/9/ Nyffeler, Urs P., Yuan-Hui Li & Peter H. Santschi, 1984. "A kinetic approach to describe trace-element distribution between particles and solution in natural aquatic systems". Geochim. Cosmochim. Acta, Vol. 48, pp. 1513-1522.

/10/ Santschi, P.H., 1988. "Factors controlling the biogeochemical cycles of trace elements in fresh and coastal marine waters as revealed by artificial radioisotopes". Limnol. Oceanogr., 33(4, part 2), pp. 848-866.

/11/ Santschi, P.H., Urs P. Nyffeler, Y.-H.Li & P. O'Hara, 1986 "Radionuclide Cycling in Natural Waters: Relevance of Scavenging Kinetics". Chapter 17 of sediment/water interaction, proceedings of 3rd international symposium, pp. 183-191.