# “The PEC model”

## ERMS Workshop,
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presented by

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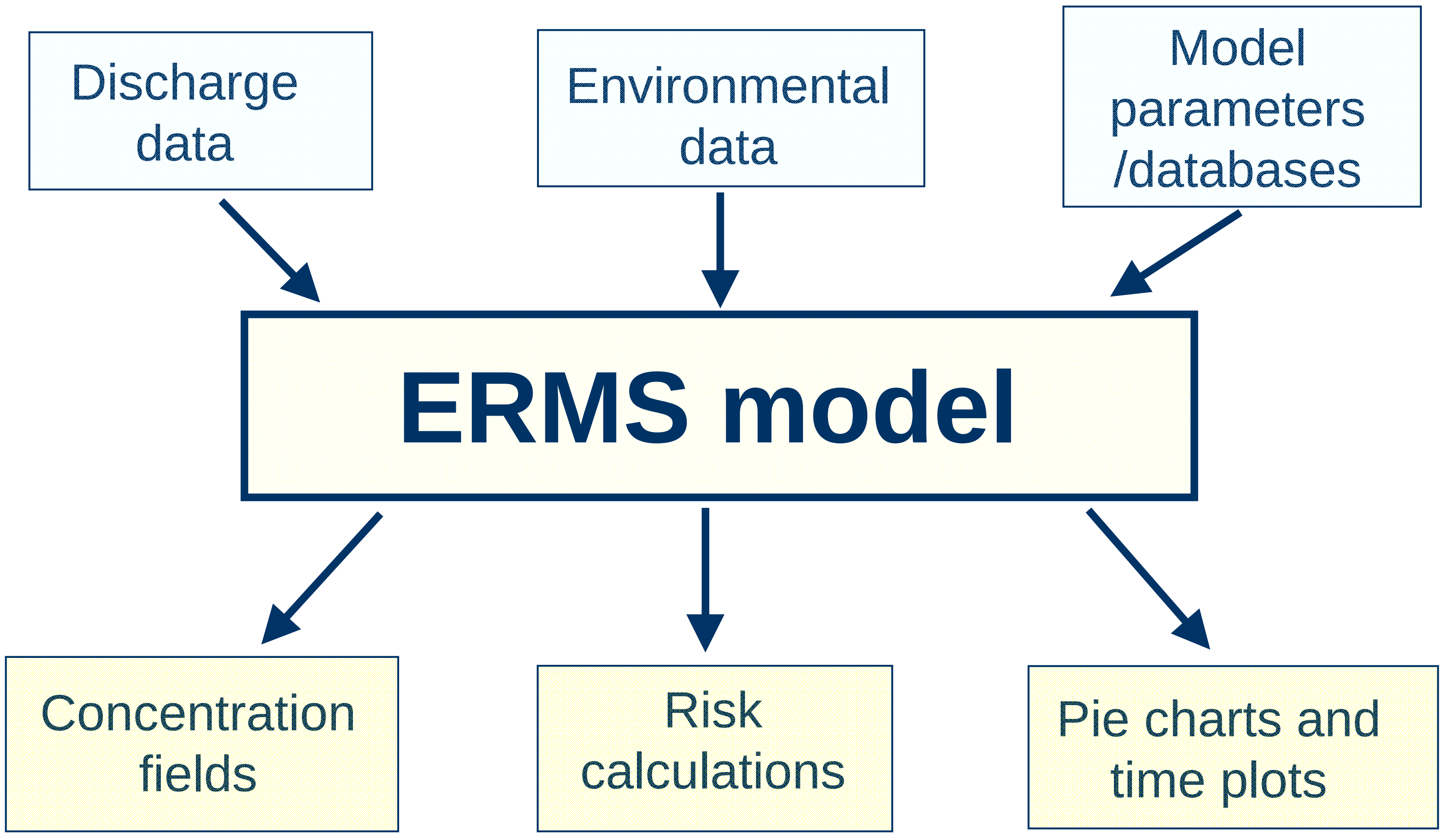
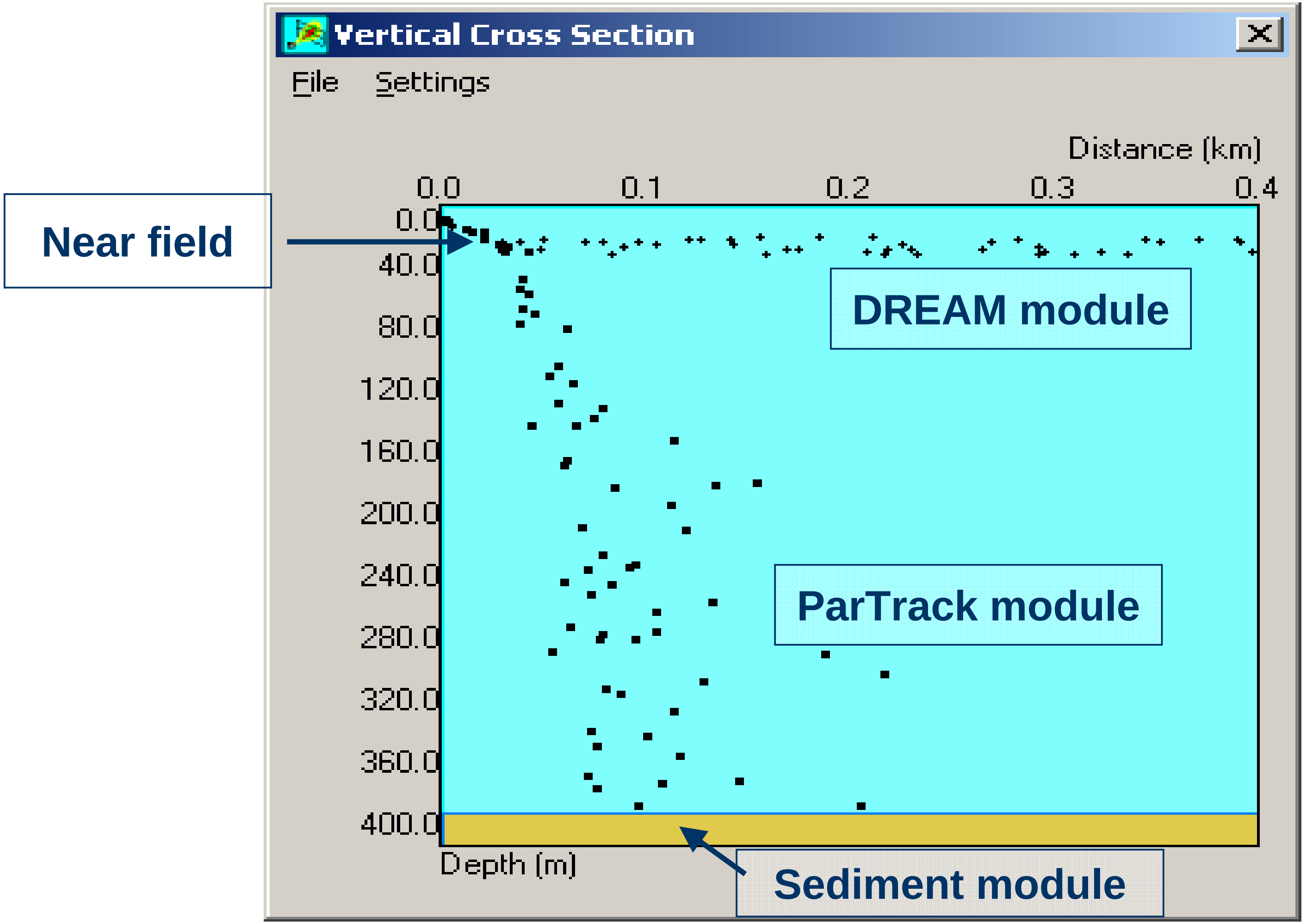
**SINTEF**

# Model structure:



# Near field plume, dissolved chemicals and settling of particles:



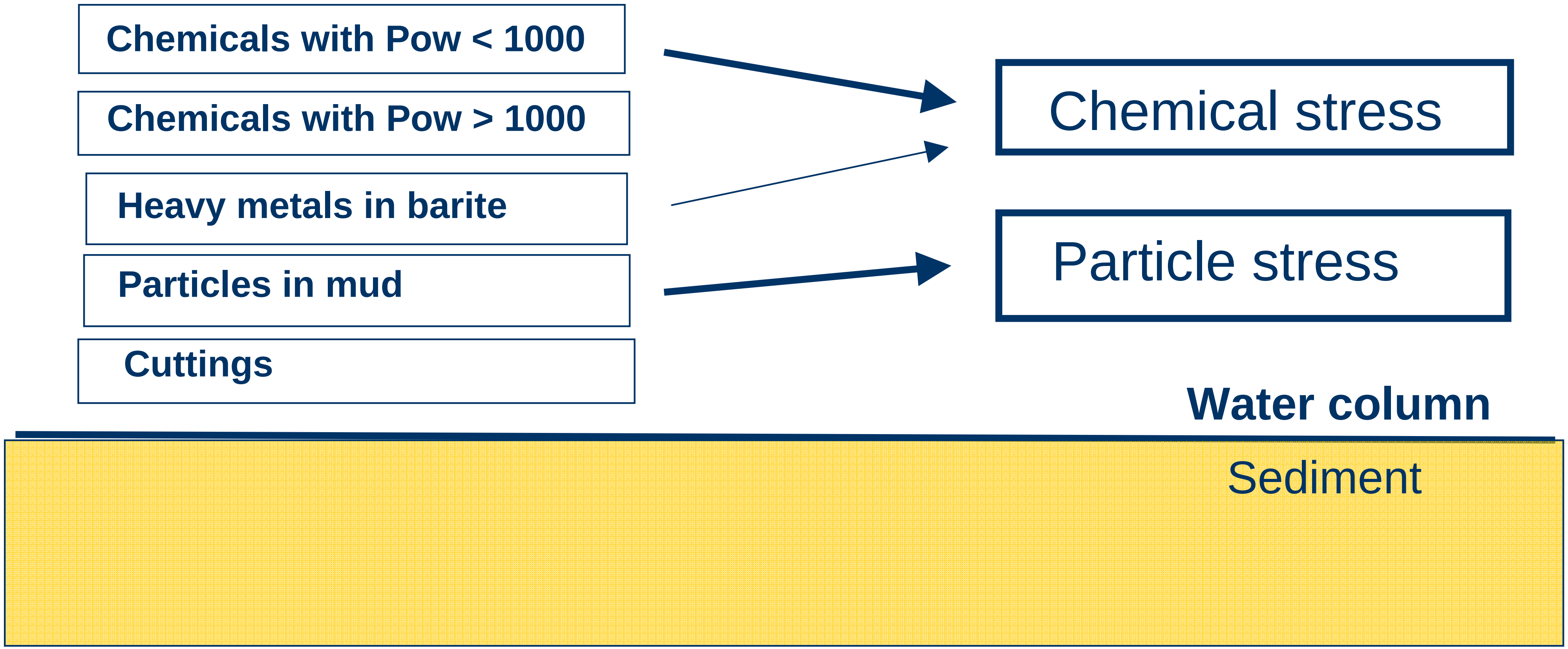
# Risk areas/volumes are calculated for:

- Water volume where PEC/PNEC > 1 for
  - Chemical stress (toxicity)
  - Particle stress in the water column (barite)

- Sediment surface area where PEC/PNEC > 1 for
  - Chemical stress (toxicity)
  - Burial
  - Change in grain size
  - Oxygen depletion

# Impact on water column:

Discharge compound: Impact:

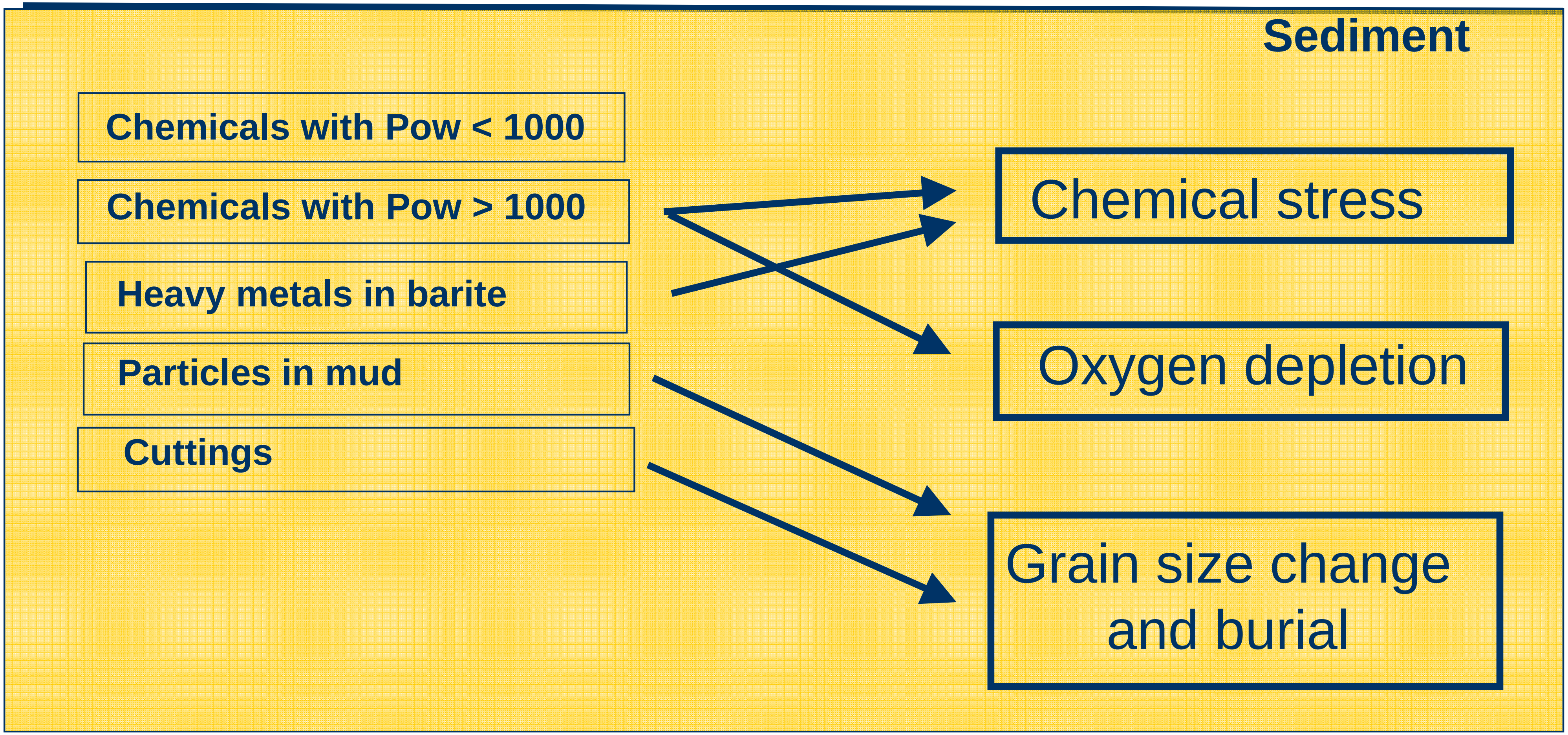


# Impact on sediment:

Discharge compound:

Impact:

Water column



# Dissolved compounds in the water column:

- **Equation 2. Calculation of local $PEC_{seawater}$ for the marine environment (ERMS approach)**
- **$PEC_{seawater} = C_{discharge} * \exp(-kt) / DILUTION$**

- *$PEC_{seawater}$ = local concentration in seawater during emission episode [$mg*l^{-1}$]*
- *$C_{discharge}$ = concentration of the substance in the discharge [$mg*l^{-1}$]*
- *k = biodegradation factor ($days^{-1}$)*
- *t = time (days)*
- *DILUTION = dilution factor [-]*

# Dissolved metals from barite in the water column:

- **Equation 4. Calculation of local PEC $_{seawater}$ for dissolved metals from barite in the marine environment (ERMS approach)**
- **$PEC_{seawater} = (C_{discharge} / DILUTION) * (FRACTION / Kp_{metal})$**

- *$PEC_{seawater}$ = local concentration in seawater of dissolved metal [mg*l$^{-1}$]*
- *$C_{discharge}$ = concentration of barite particles in the discharge [mg*l$^{-1}$]*
- *DILUTION = dilution factor for dilution of the discharge in recipient water (-)*
- *FRACTION = fraction of the metal in barite (kg metal/kg barite)*
- *$Kp_{metal}$ = partition coefficient between the metal in barite and dissolved metal*

# Partition coefficient for metals in the water column:

- Equation 5. Calculation of Kp metal (TGD approach)
  - $Kp_{metal} = C_{sol}/C_{aqu}$

- *Csol = Total available concentration in the solid phase [mg*kg-1]*
  *Caqu = Available concentration in the aqueous phase [mg*kg-1]*

# PEC for sediment (ERMS approach):

- Equation 9. Calculation of local $PEC_{sediment}$ for the marine environment (ERMS approach)
  - **$PEC_{sediment} = [1000 / RHO_{susp}] * PEC_{discharge} / DEPOSITION$**

- *$PEC_{discharge}$ = concentration in discharge pipe [mg*l-1]*
- *DEPOSITION = deposition factor calculated by the model (-)*
- *$RHO_{susp}$ = bulk density of suspended matter in sediment [kg*m-3]*
- *$PEC_{sediment}$ = predicted environmental concentration in sediment [mg*kg-1]*

# PEC for organic chemicals in sediment:

- **Equation 10. Calculation of local $PEC_{sediment}$ for organic chemicals in sediment (ERMS approach):**
  - **$PEC_{sediment} = PEC(t=0)_{sediment} * \exp(-kt) / BIOTURB$**

- *$PEC_{sediment}$ = concentration of chemical in the sediment [$mg*kg^{-1}$]*
- *$PEC(t=0)_{sediment}$ = same as above for the initial time step $t = 0$.*
- *$k$ = biodegradation factor for chemical in the sediment [$days^{-1}$]*
- *$t$ = time [days]*
- *BIOTURB = dilution factor in the sediment due to effects from bioturbation [-]*

# Partition of organic chemicals in sediment:

- Equation 11. Calculation of local pore water concentration $PEC_{porewater}$ for organic chemicals (TGD approach):
  - $\mathbf{PEC_{porewater} = [RHO_{susp} /1000] * PEC_{sediment} * Kp_{susp\text{-}water}}$

- $PEC_{porewater}$ = *concentration of chemical in the pore water* $[mg*l^{-1}]$
- $PEC_{sediment}$ = *concentration of chemical in the sediment* $[mg*kg^{-1}]$
- $RHO_{susp\text{-} water}$ = *bulk density of suspended matter* $[kg/m^{-3}]$
- $Kp_{susp\ water}$ = *suspended matter-water partitioning coefficient* $[m^3*m^{-3}]$

# Partition coefficient for organic matter in sediment:

- Equation 12. Calculation of $Kp_{susp\text{-}water}$ of non-ionic organic substances in sediment (TGD approach)
  - $\mathbf{Kp_{susp\text{-}water} = F_{oc} * K_{oc}}$
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*$K_{oc}$ = partition coefficient organic carbon-water [l*kg-1]*
*$F_{oc}$ = weight fraction of organic carbon in compartment [kg*kg-1]*

# Barite heavy metals conc. in sediment:

- **Equation 13. Calculation of local $PEC_{metal}$ for barite metals in sediment (ERMS approach):**
  - **$PEC_{metal} = PEC\ (t=0)_{sediment} * FRACTION / BIOTURB$**

- *$PEC_{metal}$ = concentration of barite metal in the sediment [$mg*kg^{-1}$]*
- *$PEC\ (t=0)_{sediment}$ = concentration of deposited barite in the sediment at t = 0 [$mg*kg^{-1}$]*
- *FRACTION = content of the metal in barite [kg metal * $kg^{-1}$ barite]*
- *BIOTURB = dilution factor in the sediment due to effects from bioturbation [-]*

# Pore water dissolved heavy metal concentration in sediment:

- **Equation 14. Calculation of local pore water concentration $PEC_{porewater}$ for barite metals (ERMS approach):**
  - $$PEC_{porewater} = [RHO_{susp} /1000] * PEC_{metal} * Kp_{metal\text{-}water}$$

- *$PEC_{porewater}$ = concentration of dissolved metal in the pore water [$mg*l^{-1}$]*
- *$PEC_{metal}$ = concentration of metal in the sediment [$mg*kg^{-1}$]*
- *$RHO_{susp}$ = bulk density of suspended matter [$kg/m^{-3}$]*
- *$Kp_{metal\text{-}water}$ = barite metal-water partitioning coefficient [$m^3*m^{-3}$]*