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TOXSWA

Improvements in TOXSWA: hourly temperatures and temperature-dependent diffusion

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Introduction

- TOXSWA calculates exposure concentrations for aquatic and sediment-dwelling organisms.
- In the current TOXSWA versions the monthly averaged temperature is used as water and sediment temperature.
- TOXSWA has been extended with options to simulate:
  a. temperature in the water and sediment using hourly terms of the energy budget of the water system (and $T_{sediment} = T_{water}$), and
  b. diffusion coefficient as a function of the water temperature and related viscosity instead of being fixed at a value reflecting a water temperature of 20°C.

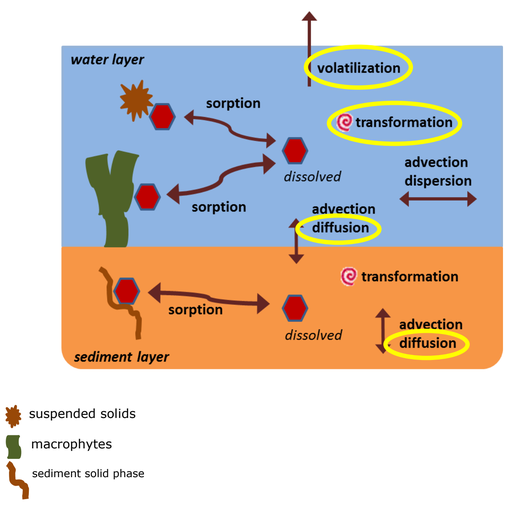


Figure 1. Processes modelled in TOXSWA. Processes affected by temperature are indicated in yellow ellipses.

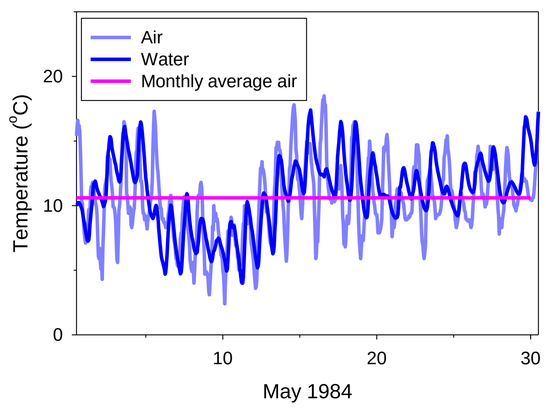


Figure 2. Temperature in water simulated by TOXSWA using hourly metereological data. The measured and monthly average air temperature are also given. Example for meteo station De Bilt, May 1984.

Objective

To evaluate the impact of the improved concepts on calculated exposure concentrations: (a) hourly water temperature values, and (b) temperature-dependent diffusion coefficient.

Effect of hourly temperature values

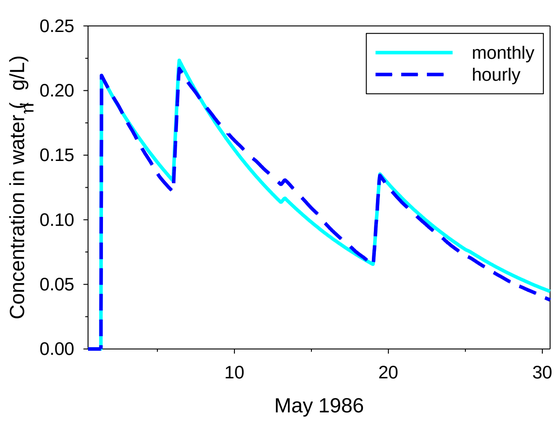


Figure 3. Effect of transformation rate as a function of hourly temperature values on concentration in water in the R1 FOCUS pond (single application of 1 kg/ha, maize, substance $DegT_{50\text{-water}}$ = 3 d, K_{om}= 38 L/kg).

- In periods with hourly temperatures below or above the constant monthly T of 11ºC (e.g. 6–13 May, or 13-20 May) concentrations are slightly lower or higher than the concentrations for T=11ºC.
- Slight effects on concentrations in water were similar in tests for effect of hourly temperatures on volatilization and diffusion (Beltman *et al*., 2017).

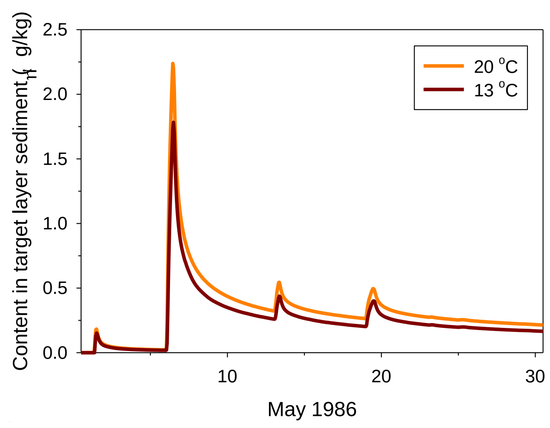
Effect of temperature-dependent diffusion coefficient

- Diffusion coefficient is function of temperature and of viscosity of water:

$$D_w = \frac{T}{T_{ref}} \frac{\eta_{w,ref}}{\eta_w} D_{w,ref}$$

D_w = diffusion coefficient in water ($m^2\ s^{-1}$)
T = ambient temperature of water (K)
T_{ref} = reference temperature (K)
η_w = dynamic viscosity of water (Pa s^{-1})
$\eta_{w,ref}$ = dynamic viscosity of water at reference temperature (Pa s^{-1})
$D_{w,ref}$ = diffusion coefficient in water at reference temperature ($m^2\ s^{-1}$) [$4.3 \cdot 10^{-5}$ m^2/d at 20ºC]

- D_w at 10ºC is 3/4 of D_w at 20ºC (30% increase of viscosity), so the exposure in sediment is a function of the water and sediment.



- R1 stream in North Europe, T in May is 13ºC.
- $D_w = 3.5 \cdot 10^{-5}$ m^2/d.
- Decreased penetration into sediment, because 13ºC < 20ºC
- PEC-sediment is 18% lower.

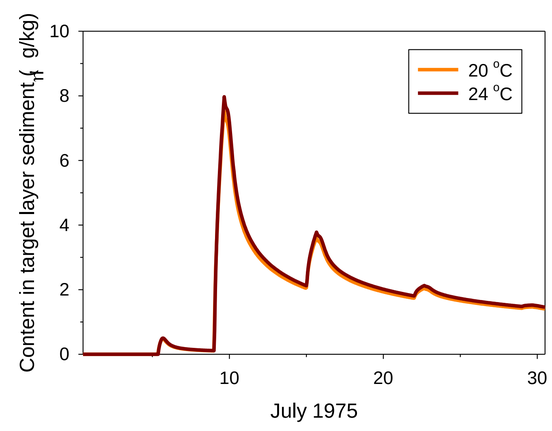


Figure 4. Effect of diffusion on content in sediment in the R1 (upper graph) and R3 (lower graph) FOCUS streams (single application of 1 kg/ha in maize, substance K_{om} = 38 L/kg, $DegT_{50\text{-water}}$= 24 d, $DegT_{50\text{-sediment}}$= 1000 d)

- R3 stream in South Europe, T in July is 24ºC.
- $D_w = 4.8 \cdot 10^{-5}$ m^2/d.
- Increased penetration into sediment, because 24ºC > 20ºC
- PEC-sediment is 5% higher.

Conclusions

a. Introduction of temperature simulated on an hourly basis into the TOXSWA model instead of a constant monthly temperature slightly changes the exposure of aquatic organisms.
b. Introduction of a temperature-dependent diffusion coefficient changes the exposure concentrations of sediment dwelling organisms up to approximately 20%.

References

Beltman, W.H.J, P.I. Adriaanse, C.M.J. Jacobs and H.M. Mulder, 2017. Temperature in water and sediment in the pesticide model TOXSWA. Implementation report. Wageningen, Wageningen Environmental Research, Report 2794.

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