TOXSWA simulates metabolite formation in water and in sediment

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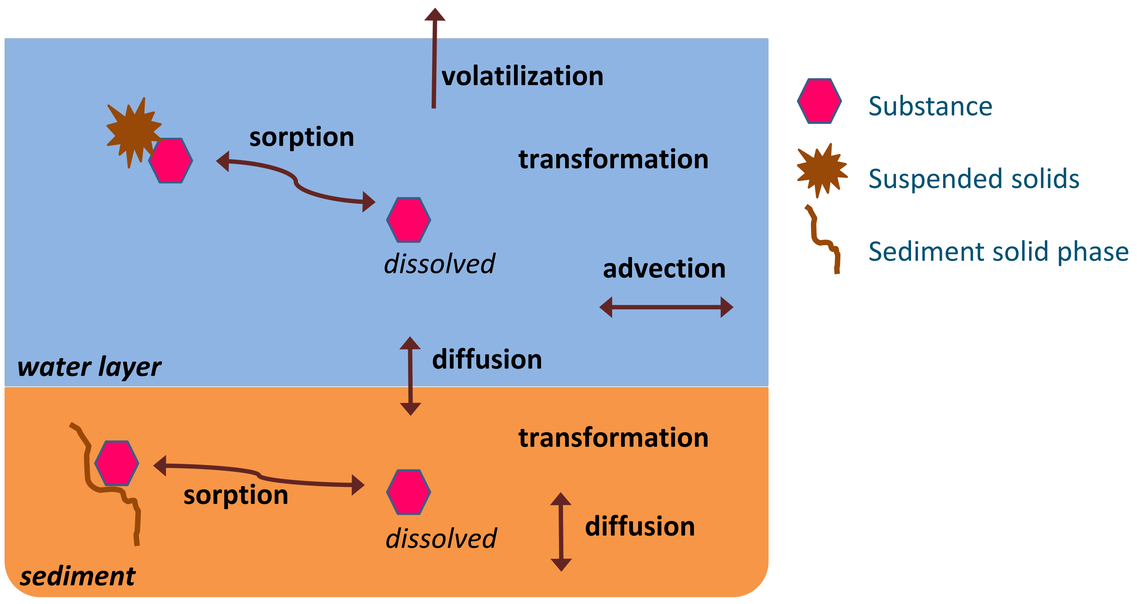
Introduction

If pesticide metabolites are toxic and formed in sufficient quantities, they may pose a risk for the aquatic ecosystem or for drinking water production from surface water. FOCUS_TOXSWA (v4.4.2) calculates exposure concentrations of parent and of metabolites formed in water and in sediment. Example simulations are done for FOCUS R1 pond. Runoff is calculated by FOCUS_PRZM 3.1.1.

Processes modelled in FOCUS R1 pond



Input for calculations

Insecticide, and its metabolite formed in water

Fungicide, and its metabolite formed in sediment

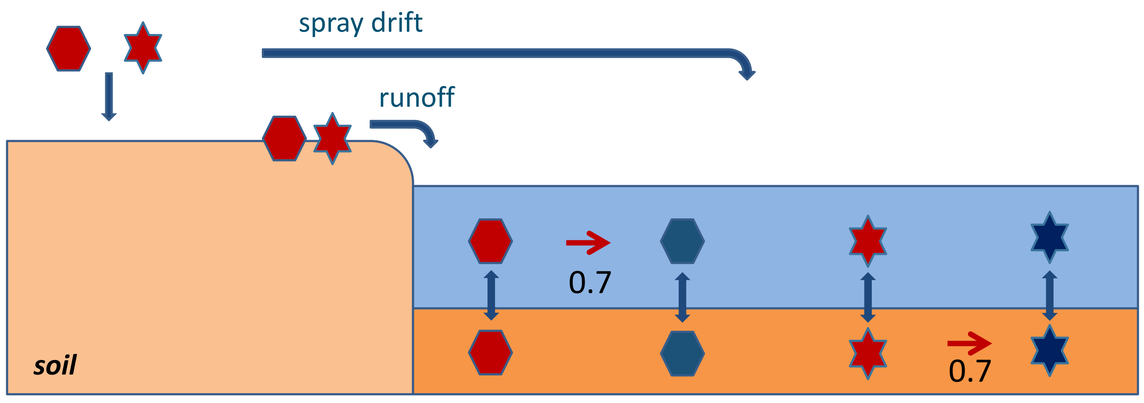


Table 1 Application rates and substance properties

Applications (g/ha)	70 + 105		750	
K_{om} (L/kg)	100	10	1000	10
DegT50 (d) soil	100	not relevant	50	not relevant
DegT50 (d) water	5	100	10	100
DegT50 (d) sediment	100	100	20	100

Metabolite formed in water

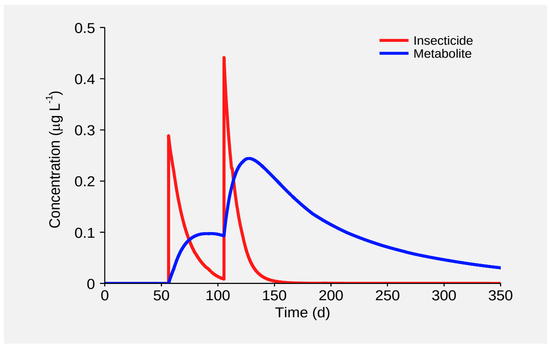


Figure 1. Concentration in water. Applications day 57 and day 107.

Insecticide concentration in water
- decreases rapidly due to its short half-life (5 d).

Metabolite concentration in water
- increases rapidly due to rapid transformation of insecticide,
- and thereafter decreases slowly due to its long half-life (100 d).

Metabolite formed in sediment

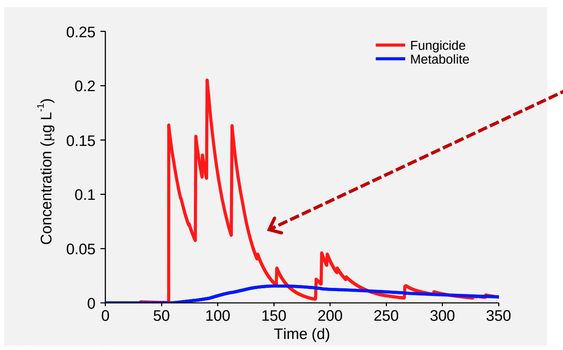


Figure 2. Concentration in water.

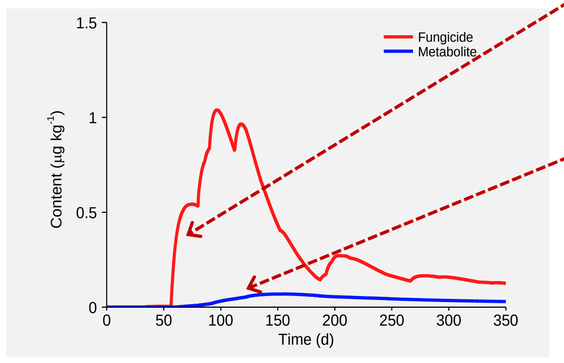


Figure 3. Content in sediment.

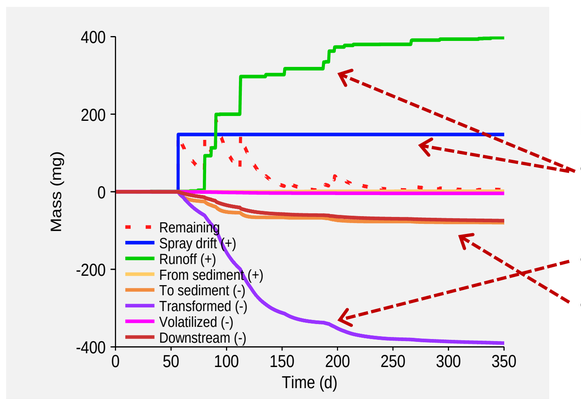


Figure 4. Mass balance fungicide in water.

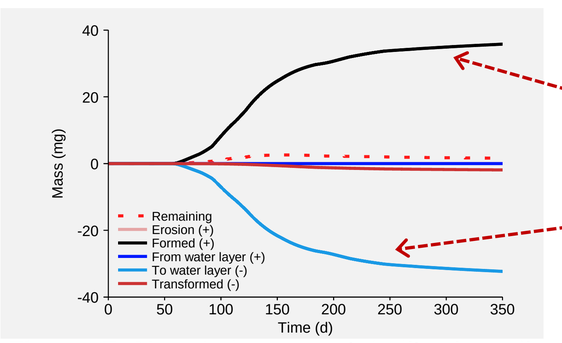


Figure 5. Mass balance metabolite in sediment.

Fungicide concentration in water
- shows peaks after spray drift event at day 57 and several runoff events,
- decreases rapidly due to its short half-life (10 d).

Fungicide content in sediment
- increases due to diffusion from water layer.

Metabolite content in sediment
- increases because fungicide is rapidly transformed (half-life 20 d).

Metabolite concentration in water
- increases from day 70 onwards (Fig. 2), due to diffusion from sediment.

Fungicide mass in water
- enters by runoff events and by spray drift,
- leaves mainly by transformation,
- leaves in equivalent amounts by downstream outflow and by diffusion to sediment.

Metabolite mass in sediment
- is rapidly formed due to transformation of fungicide diffused from water layer,
- diffuses almost fully towards the water layer.

Conclusion

The TOXSWA model now simulates the formation and behaviour of metabolites in water and in sediment.

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[1]Simulations also published in EFSA (Scientific Panel on Plant protection products and their Residues), 2013. Appendices to Scientific Opinion. Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters.