Testing the TOXSWA model against outdoor ditch measurements

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Overview

• Introduction to TOXSWA model
• Importance hydrological submodel
• Field tests: # prosulfocarb # chlorpyrifos
• Conclusions
TOXSWA model

- Behaviour of pesticides in small surface waters

- Main use:
  - registration in NL (June 1999, v 1.2)
  - Annex I of EU (May 2003, v 1.1.1 and 2.2.1)

- Available via:
  - http://www2.alterra.wur.nl/ (v 1.2)
  - http://viso.ei.jrc.it/focus/ (v 2.2.1)

Hydrology in TOXSWA

- Simplified hydrological submodel

- Watercourse embedded in catchment

- Water conservation:

  Accumulation =
  \[ \text{inflow} - \text{outflow} + \text{lateral inflow} \]

  \[ \text{seepage} \]

  N.B. 1. inflow from neighbouring field plus upstream area
  2. behaviour field = behaviour upstream area
Hydrology in TOXSWA (2)

- Transient hydrology: $Q(x,t)$ and $h(t)$ only
- Water depth $h(t)$ via $Q_{out} = 1.7 \cdot w \cdot h_2^{3/2}$ as lower boundary condition watercourse

$Q = \text{discharge}$  
$w = \text{width crest}$  
$h_1 = \text{height crest weir}$  
$h_2 = \text{water depth on crest}$  
$h = h_1 + h_2$

- Example R1 stream

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**R1 stream**

Graph showing:
- Rain (mm/d) over time (d) from 1 Oct 1978
- Runoff (mm/d) over time (d) from 1 Oct 1978
Pesticide behaviour in TOXSWA

- Mass conservation:

  \[ \text{Accumulation} = \text{input} - \text{output} - \text{sinks} \pm \text{exchange} \]

  # input = spray drift + either drainfluxes or runoff/erosion (neighbouring field + upstream area)
Processes in water and sediment

- **Water plants**
- **Suspended solids**
- **Sed. material**
- **Water phase**
- **Liquid phase**

- **Transport:** advection, dispersion, diffusion
- **Transformation**
- **Sorption**
- **Volatilization**
- **Advection (up/downward seepage)**
- **Diffusion**

Upstream area: 100 ha, 20 ha treated
Testing TOXSWA model

- testing model output against field measurements
- target variable: $c(x,t)$ in water (and sediment)
- domain: single watercourse (no network)
- no serious tests available
Importance hydrological submodel (1)

- Tracer in FOCUS ditch D1
- FOCUS scenario:
  1 ha neighbouring field
  2 ha upstr. not treated

- Dilution factor 3 as expected

Importance hydrological submodel (2)

- Tracer in FOCUS ditch D1
- Modified FOCUS scenario:
  1 ha neighbouring field
  2 ha upstr. treated

- $c(t)$ in ditch $\quad c(t)$ in drain, (except when drainflow is very low)
- So, in ditch:
  $c(t)$ strongly driven by scenario characteristics
Importance hydrological submodel (3)

- Tracer in FOCUS stream R1
- FOCUS scenario:
  1 ha neighbouring field
  100 ha upstr. area
  of which 20 ha treated

- So, dilution factor 5 expected

Importance hydrological submodel (4)

- Tracer in FOCUS stream R1

<table>
<thead>
<tr>
<th>Event</th>
<th>Dilution</th>
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</thead>
<tbody>
<tr>
<td>1</td>
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<td>5</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>7</td>
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![Runoff graph]

![Stream graph]
Tracer in stream R1 (cont)

- Water volume R1 stream: $0.42 \times 1.0 \times 100 = 42 \text{ m}^3$
- All events (except 2 and 4): stream water replaced
- Event 2 and 4: only 9 and 0.5 m³ from 100 ha catchment

<table>
<thead>
<tr>
<th>Event</th>
<th>Dilution TOXSWA</th>
<th>Predicted dilution</th>
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<tbody>
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<tr>
<td>6</td>
<td>7</td>
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</tr>
</tbody>
</table>

*So, c(t) is strongly driven by scenario characteristics (100 ha upstream area of which 20 ha treated), except in case of very low runoff volumes*
Conclusion for hydrology

For main uses of TOXSWA model (FOCUS sw scenarios):
Change of target variable $c(x,t)$ from input (drains/runoff) to output (end watercourse) is predictable from scenario characteristics (except for low incoming water volumes)

So, for testing the TOXSWA model:
concentrate on role processes

\textit{N.B. Testing TOXSWA testing the FOCUS sw scenarios !}

Field tests

- Ditches: 40*1.65*0.50 m
- Stagnant
- Spray drift appln
- $c(t)$ in water, sediment, macrophytes

Prosulfocarb April May 2002
Chlorpyrifos May Sept 1990
Prosulfocarb

- Herbicide in cereals, potatoes
- Use rate 3 4 kg/ha
- Appln 22 April 2002
- Shielded spray boom (5% of 3.2 kg/ha)
- $C_{ini} = 76$ g/L (1 ditch)
- Water and sediment sampled as f(t)

Prosulfocarb

- Standard lab tests:
  - $K_{om} = 1018$ L/kg, 3 soils
  - $DT_{50,system} = 335$ d (sys 1)
    - $= 147$ d (sys 2)

Estimation of separate degradation rate in water and sediment not possible (see poster Ter Horst et al).
So, use average $DT_{50,system} = 204$ d
Experimental ditches (1)

Simulation A
Input from standard lab tests

\[ DT_{50,\text{water}} = DT_{50,\text{sediment}} = DT_{50,\text{system}} = 204 \text{ d} \]

\[ K_{om} = 1018 \text{ L/kg} \]

test model output against field

test acceptable?

Simulation B

DT\textsubscript{50}'s optimised by PEST

\[ K_{om} \text{ from standard lab tests} \]

\[ DT_{50,\text{water}} = 10 \text{ d (4 to 24 d)} \]

\[ DT_{50,\text{sediment}} = 178 \text{ d (4749 to 5106 d)} \]

\[ K_{om} = 1018 \text{ L/kg (fixed)} \]
test model output against field

**Simulation C**

Both $K_{om}$ and $D_{T50}$’s optimised by PEST

$D_{T50,\text{water}} = 6 \text{ d} (4 \text{ to } 9 \text{ d})$

$D_{T50,\text{sediment}} = 13 \text{ d} (3 \text{ to } 24 \text{ d})$

$K_{om} = 7185 \text{ L/kg} (4053 \text{ to } 10317 \text{ L/kg})$

Conclusions: prosulfocarb in experimental ditches

- For calibrated $D_{T50}$’s and $K_{om}$ perfect fit, so concepts regarding process descriptions not disqualified

- Not possible to describe behaviour prosulfocarb in field on basis of standard lab tests (conditions not site specific)
Chlorpyrifos

- Insecticide, widely used
- Appln 8 May 1990  (Shielded spray boom)
- $C_{\text{ini}} = 40 \text{ g/L (2 ditches)}$
- Water, sediment and macrophyte sampled as $f(t)$

Chlorpyrifos

- Site specific input
  
  # $DT_{50,\text{water}} = f(\text{pH})$  
  # $DT_{50,\text{water}} = 45 \text{ d}$  
  # $DT_{50,\text{sediment}} = 181 \text{ d}$  
  # $K_d = 630 \text{ L/kg}$ (om ?)  
  # $K_{mp} = 1980 \text{ L/(kg dry mp)}$
test model output against field

- Agreement very moderate
- Very rapid initial decline not simulated by TOXSWA, nor peak in sediment

TOXSWA: on conservative side

water

Volatilisation most important dissipation process, probably higher than simulated:
# no ideal mixing 1st day
# $T_{8\ May} > 15 ^\circ C$ (monthly mean)

sed.
test model output against field

- What if:
  - # Volatilisation 1st 10 h
    - 20\% higher:
      - ( 5 cm water instead of 50 cm
        - 20 °C instead of 15 °C)
      - # K_{em} halved
  - Agreement improved,
    so part of disagreement
    may be explained

Conclusions: chlorpyrifos in experimental ditches

- Model concepts should correspond to experiment
  - # concept of 1 water layer ideally mixed
    - microlayer cpf
    - > concept of one water layer possibly underestimates
      - volatilisation
  - # simulated monthly mean T
    - T at first hot day
    - > underestimation of rapid decline during first day
Overall conclusions

Regarding hydrology:
• For main uses of TOXSWA model (FOCUS sw scenarios):
  Dilution produced by TOXSWA from input (drains/runoff) to output (end watercourse) is predictable from scenario characteristics

Regarding processes:
• Model concepts not disqualified
• Input from standard lab tests cannot describe behaviour in field (prosulfocarb)
• Model concepts should correspond to experiment (chlorpyrifos)
• Need for number of high quality field data sets for testing TOXSWA

Welcome to any comments and questions