Testing the TOXSWA model against outdoor ditch measurements

TOXSWA

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Overview

TOXSWA

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

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TOXSWA model

TOXSWA

- 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)

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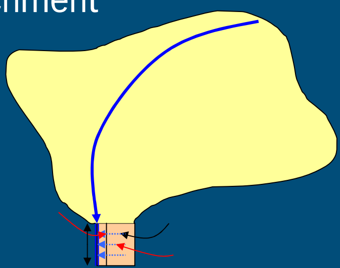
Hydrology in TOXSWA

- Simplified hydrological submodel
- Watercourse embedded in catchment



- Water conservation:

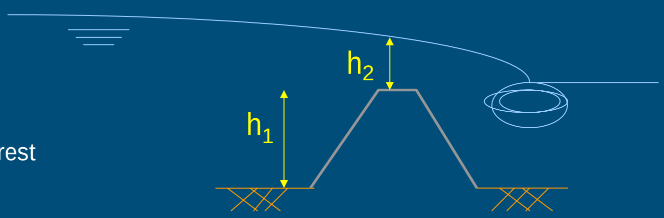
Accumulation =
inflow – outflow + lateral inflow   seepage

N.B. 1. inflow from neighbouring field plus upstream area
2. behaviour field = behaviour upstream area

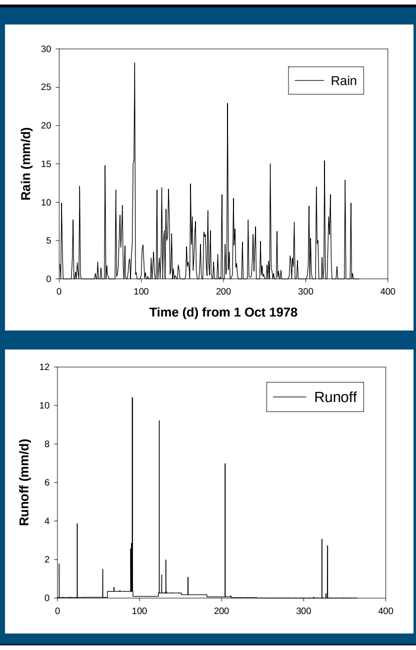
Hydrology in TOXSWA (2)

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

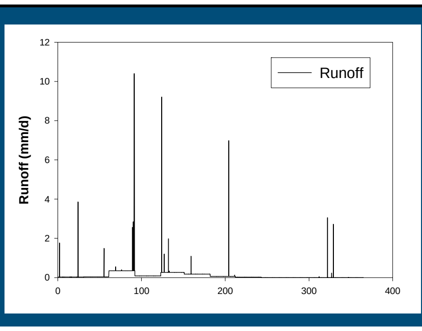
Q = discharge
w = width crest
h_1 = height crest weir
h_2 = water depth on crest
$h = h_1 + h_2$



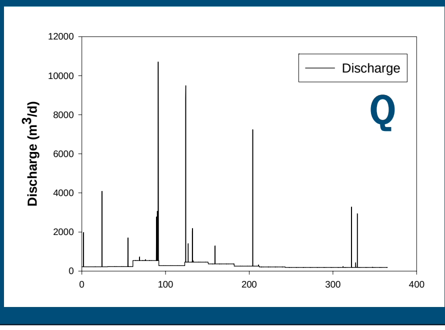
- Example R1 stream

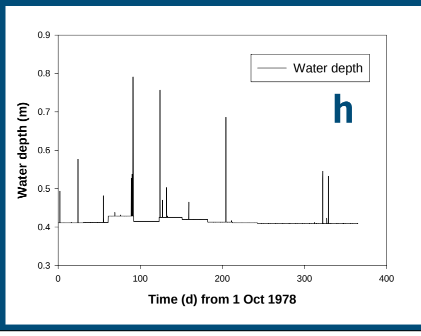


R1 stream



R1 stream:
Discharge Q(t) and
water depth h(t)





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Pesticide behaviour in TOXSWA

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• Mass conservation:

Accumulation = input – output – sinks ± exchange

input = spray drift + either drainfluxes
or runoff/erosion
(neighbouring field + upstream area)

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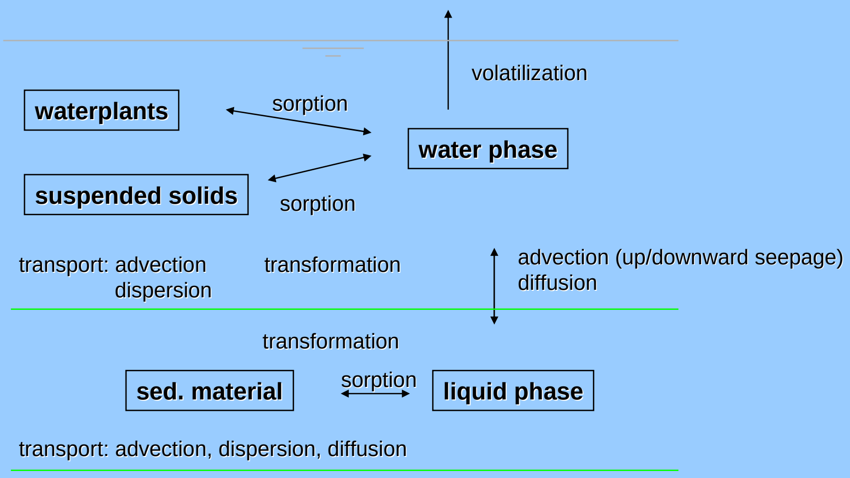
Processes in water and sediment



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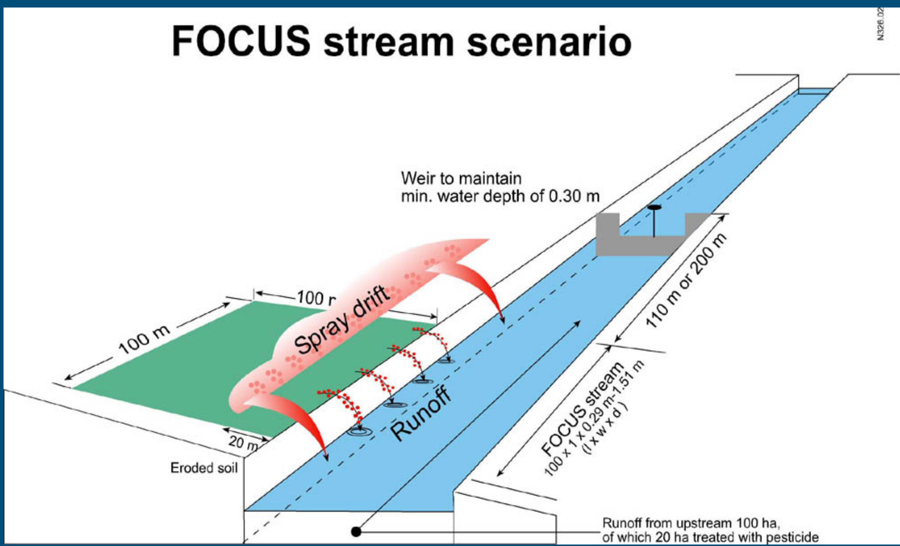

Upstream area: 100 ha, 20 ha treated

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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

Developing and testing:

problem

conceptual model

mathematical model

computer program

input parameters from lab

field experiments

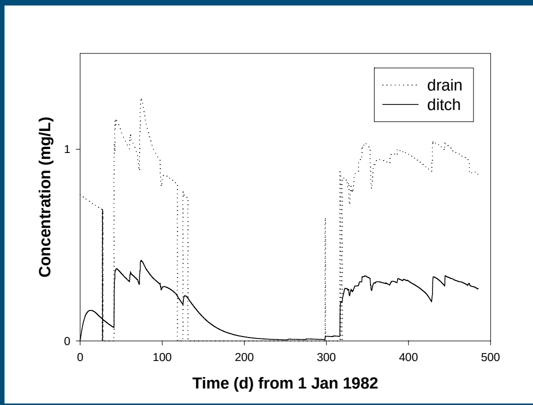
test model output against field

test acceptable ? → check all steps once again

apply model

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

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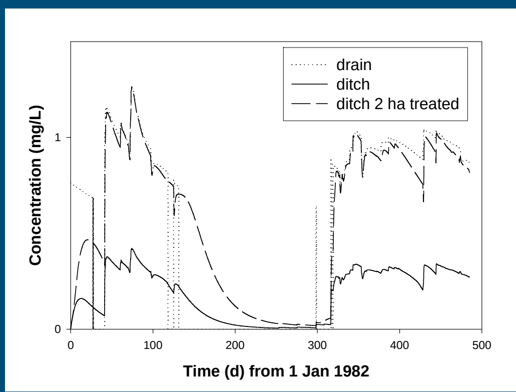
Importance hydrological submodel (2)

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



- c(t) in ditch   c(t) in drain,
  (except when drainflow is
  very low)
- So, in ditch:
  c(t) strongly driven by
  scenario characteristics

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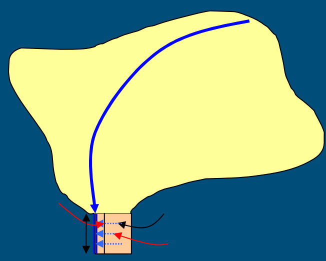
Importance hydrological submodel (3)

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

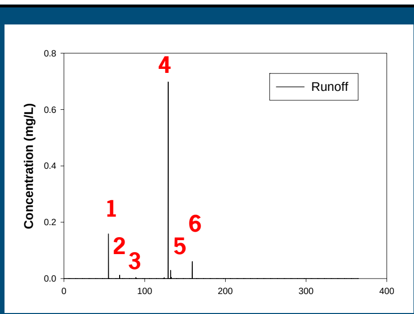


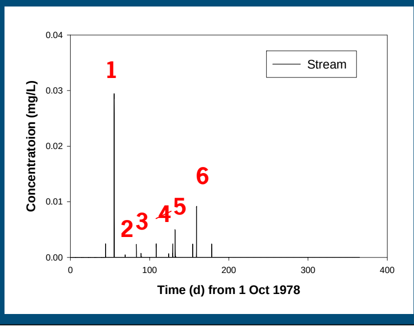
- So, dilution factor 5 expected

Importance hydrological submodel (4)

- Tracer in FOCUS stream R1

Event	Dilution
1	6
2	30
3	6
4	970
5	6
6	7





Tracer in stream R1 (cont)

- Water volume R1 stream: 0.42*1.0*100 = 42 m^3
- All events (except 2 and 4): stream water replaced
- Event 2 and 4: only 9 and 0. 5 m^3 from 100 ha catchment

Event	Dilution TOXSWA	Predicted dilution
1	6	5
2	30	25
3	6	5
4	970	420
5	6	5
6	7	5

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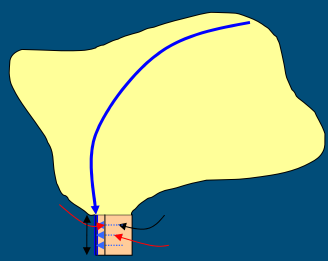
Tracer in stream R1 (cont)

- 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



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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

N.B. Testing TOXSWA   testing the FOCUS sw scenarios !

Field tests

test model output against field

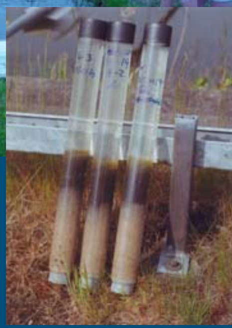
- Ditches: 40*1.65*0.50 m
- Stagnant
- Spray drift appln
- c(t) in water,
  sediment,
  macrophytes

Prosulfocarb April May 2002
Chlorpyrifos May Sept 1990

Prosulfocarb

field experiments

- 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)



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Prosulfocarb

input parameters from lab

- 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

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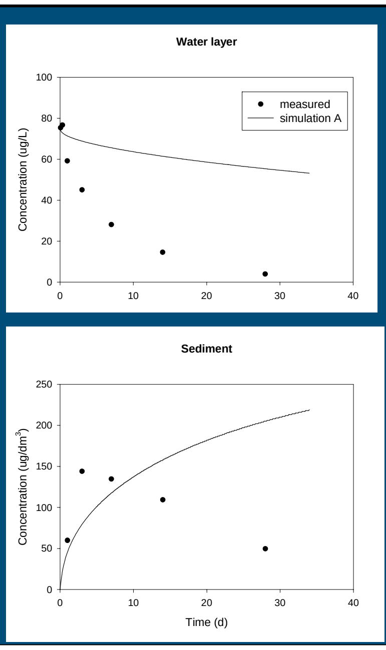

test model output against field

test acceptable ?

Simulation A

Input from standard lab tests

$DT_{50,water}$ = $DT_{50,sediment}$ = $DT_{50,system}$ = 204 d

K_{om} = 1018 L/kg

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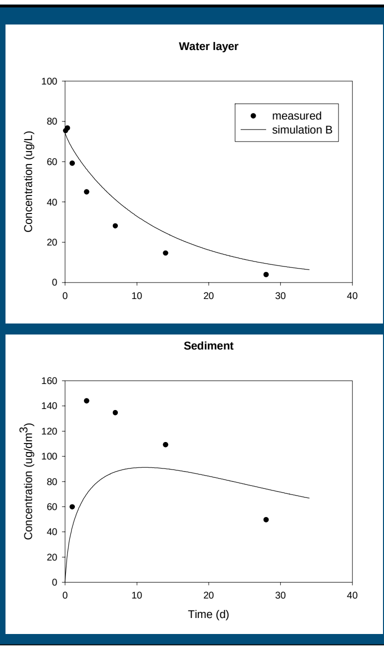

test model output against field

test acceptable ?

Simulation B

DT_{50}'s optimised by PEST
K_{om} from standard lab tests

$DT_{50,water}$ = 10 d (4 to 24 d)
$DT_{50,sediment}$ = 178 d (4749 to 5106 d)

K_{om} = 1018 L/kg (fixed)

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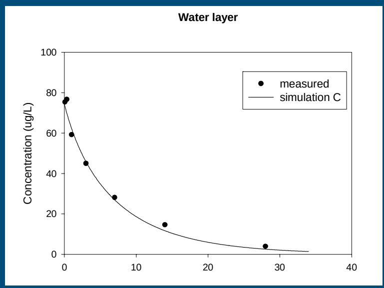

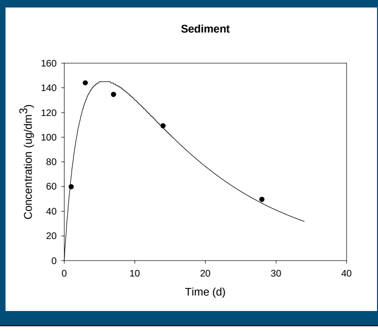

test model output against field

test acceptable ?

Simulation C

Both K_{om} and DT_{50}'s optimised by PEST

$DT_{50,water}$ = 6 d (4 to 9 d)
$DT_{50,sediment}$ = 13 d (3 to 24 d)

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

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test acceptable ?

Conclusions: prosulfocarb in experimental ditches

- For calibrated DT_{50}'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)

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Chlorpyrifos

field experiments

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

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Chlorpyrifos

input parameters from lab

- Site specific input

$DT_{50,water}$ = f (pH)   (20 °C, dark)
$DT_{50,water}$ = 45 d   for exp.ditches (pH = 8 9)

$DT_{50,sediment}$ = 181 d (10 °C, dark)

K_d = 630 L/kg (om ?)

K_{mp} = 1980 L/(kg dry mp)

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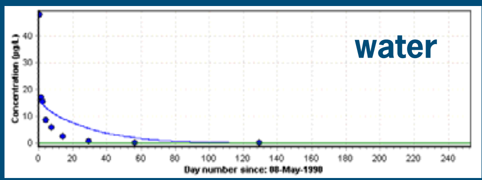
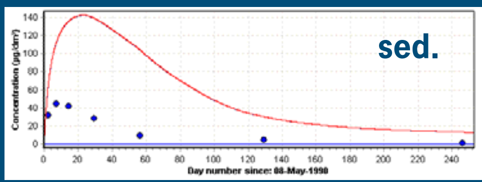
test model output against field





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

•TOXSWA:
on conservative side

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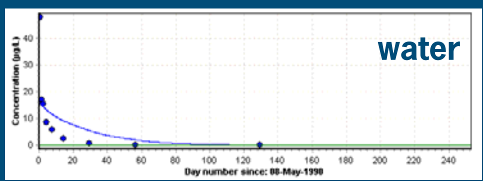
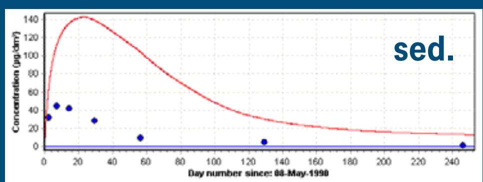
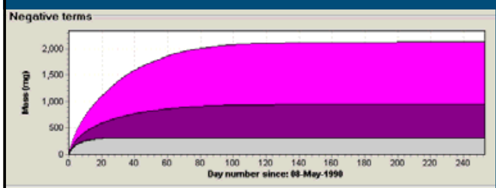
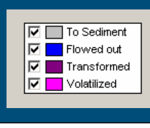
test model output against field







- Cpf in microlayer for first 10 h
- Volatilisation most important dissipation process, probably higher than simulated:
  # no ideal mixing 1st day
  # $T_{8\ \mathrm{May}}$ > 15 °C (monthly mean)



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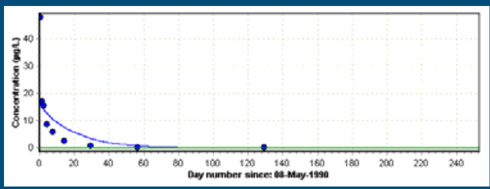
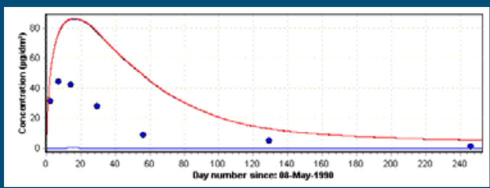
test model output against field





- What if:

Volatilisation 1st 10 h
20* higher:
(5 cm water instead of 50 cm
20 °C instead of 15 °C)
K_{om} halved

- Agreement improved, so part of disagreement may be explained

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test acceptable ?

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

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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

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Welcome to any comments and questions

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water sed.

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