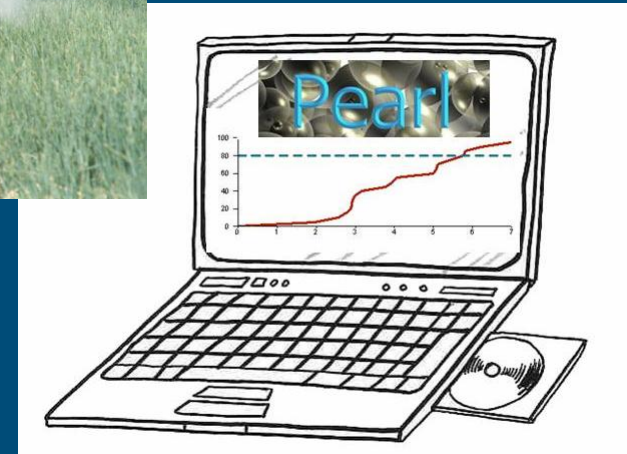


Pesticide Fate Models

Principles

Mechteld ter Horst,
(slightly adapted and presented
by Paulien Adriaanse)



Alterra, Wageningen University and
Research Centre, the Netherlands

Outline of presentation

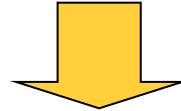
1. Introduction
2. What is a model and why modelling?
3. Definitions

1. Introduction

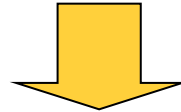
- An overall risk assessment consists of several risk assessments.
- For each protection goal a risk assessment is done
- Every risk assessment for each protection goal contains an exposure assessment

1. Introduction

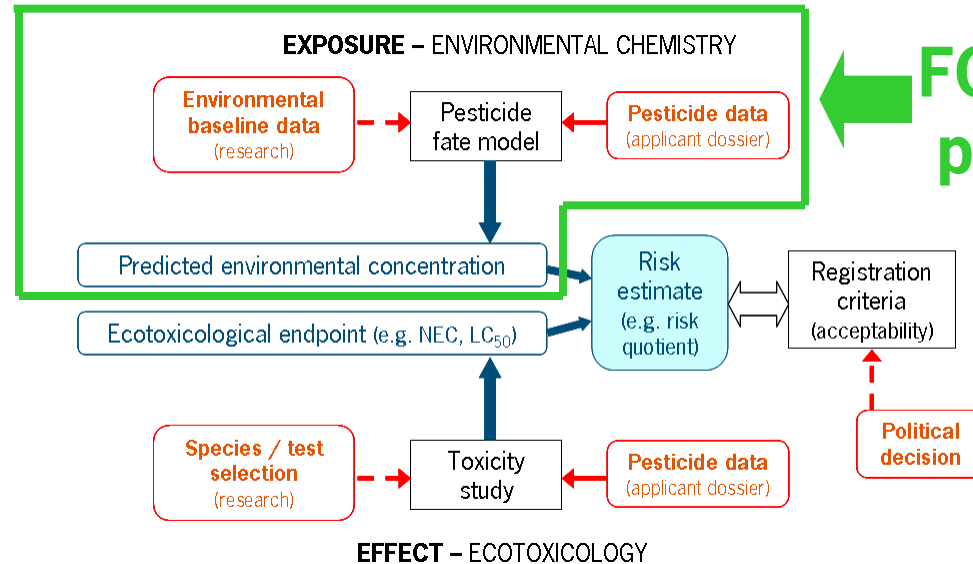
Overall Environmental Risk Assessment



Detailed protection goal



Risk Assessment for each protection goal



1. Introduction

Several models are available to calculate the exposure of each protection goal, e.g.

- Aquatic organisms
- Birds
- Persistence in soil
- Bees
- Groundwater

1. Introduction

Presentation restricted to exposure in:

- groundwater
- surface water



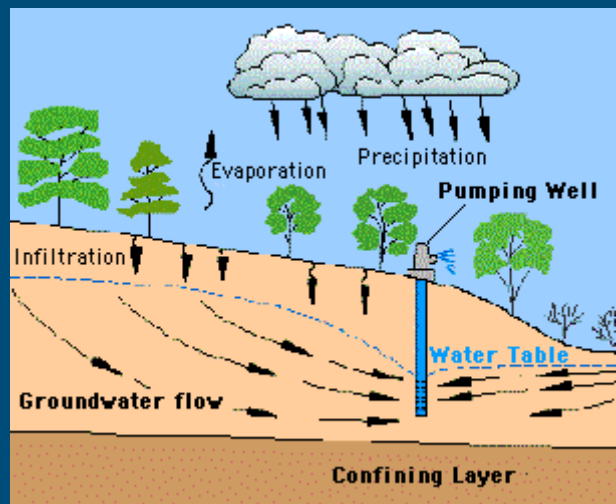
Outline of presentation

1. Introduction
2. What is a model and why modelling?
3. Definitions

2. What is a model and why modelling?

Model: simplified representation of reality

Workshop: representation of essential aspects of a system, whereby knowledge is presented in an useable form

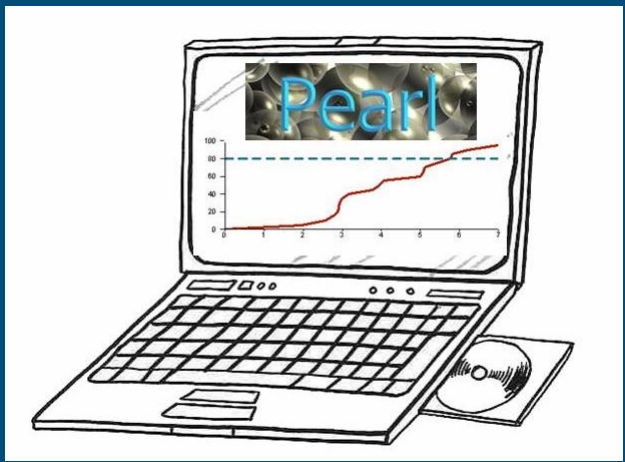


System

Flow equation:

$$\frac{\partial \theta}{\partial t} = C(h) \frac{\partial h}{\partial t} = \frac{\partial \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]}{\partial z} - S(h)$$

Knowledge = conceptual model + mathematical model



Usable form: computer program = the model

2. What is a model and why modelling?

- Alternative are measurements
 - expensive and slow
 - large variation in soils, weather (EU, Ethiopia)
 - > 100 pesticides registered (in EU, what about Ethiopia ?)
- Advantage of modelling:
 - cheap and fast
 - knowledge from one pesticide applicable to others
 - effects of other conditions
 - based on laboratory studies (available in dossiers)

Outline of presentation

1. Introduction
2. What is a model and why modelling?
3. Definitions

3. Definitions: Simple model

- Simple concepts
 - Few processes included
 - Limited number of relations between processes
- Simple mathematics
 - Calculations can be done with a calculator (analytically)
- Need only a few input parameters
- Usually short run times

3. Definitions: Complex model

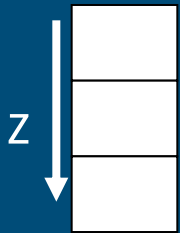
- Complex concepts
 - Many processes included
 - Many relations between processes
- Complex mathematics
 - Calculations are too complex for a calculator (numerical)
- Many input parameters
- Long(er) run times

3. Definitions: Mathematics

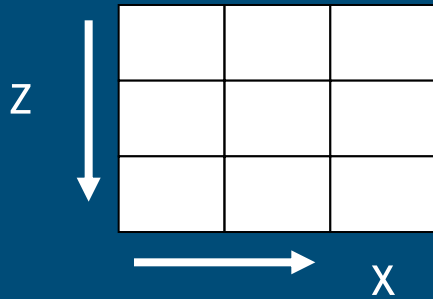
- Analytical model: Gives exact solutions to simplified mathematical forms of differential equations.
- Numerical model: Uses interpolation techniques to solve differential equations which cannot be solved analytically

3. Definitions: Dimensions

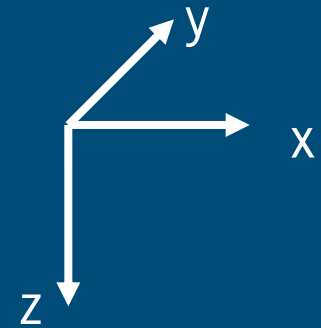
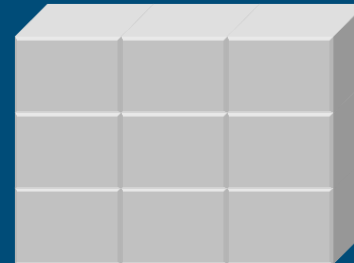
1D,



2D,



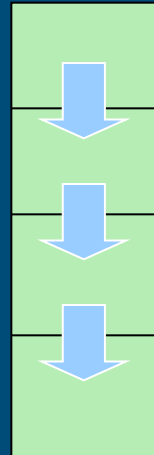
3D model:



3. Definitions: Pesticide leaching models

Specific for water flow in soil!

1. Physically based model:

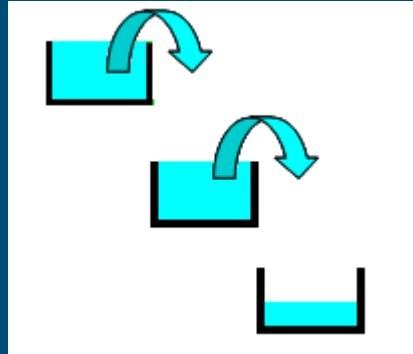


Water flow driven by water potentials (complex)

Flow equation:

$$\frac{\partial \theta}{\partial t} = C(h) \frac{\partial h}{\partial t} = \frac{\partial \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]}{\partial z} - S(h)$$

2. Compartment model:



Water flow driven by water storage (simple)

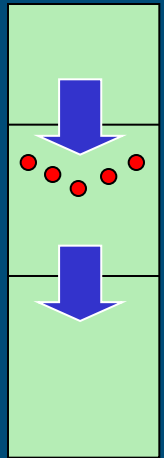
Tipping bucket approach

3. Definitions: Pesticide leaching models

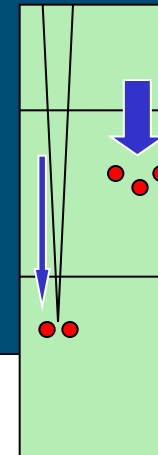
Specific for pesticide transport in soil!

Pesticide leaching models are divided into 2 categories:

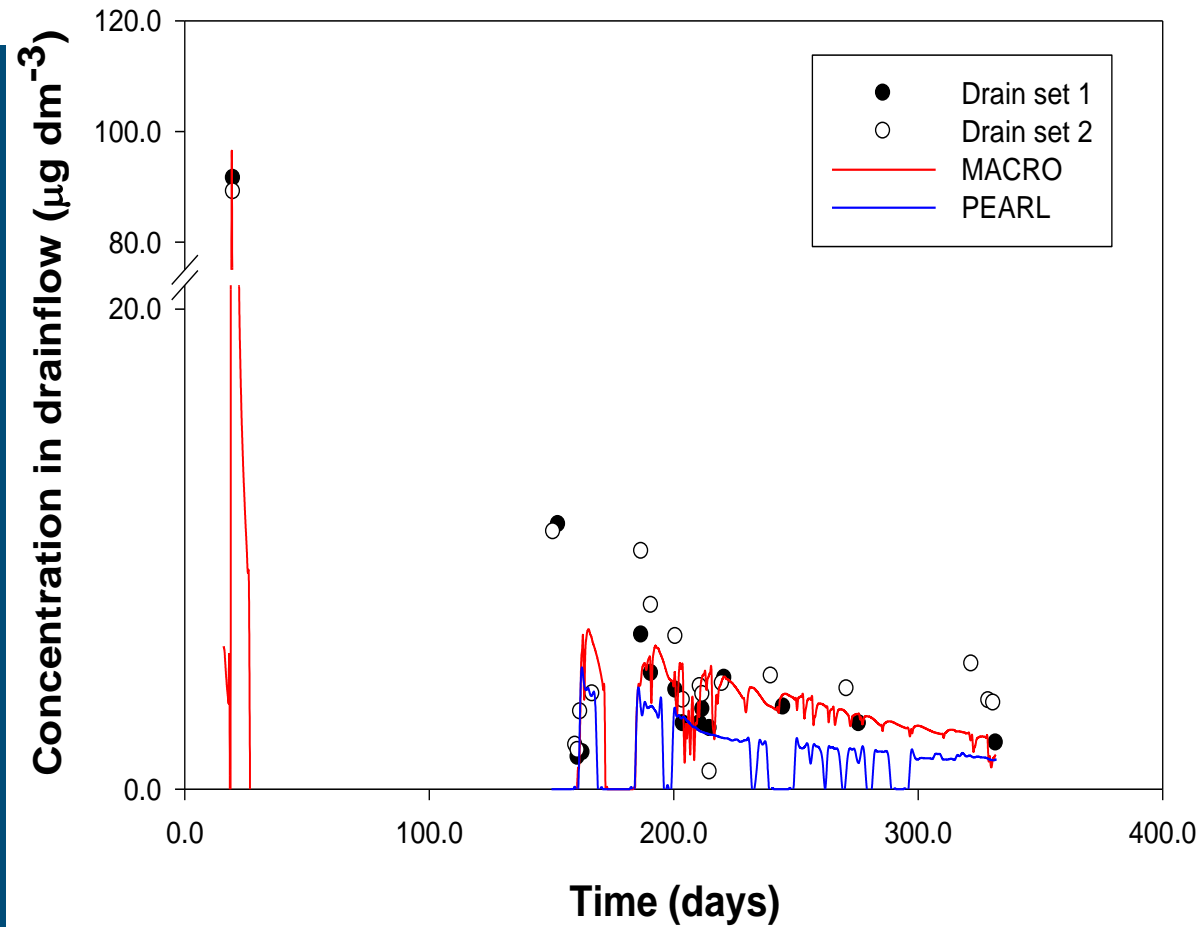
1. Chromatographic model: based on the convection/dispersion equation: tracers flow through soil at rates that are normally distributed



2. Preferential flow model: more rapid flow for part of the soil moisture and rapid transport of the pesticide



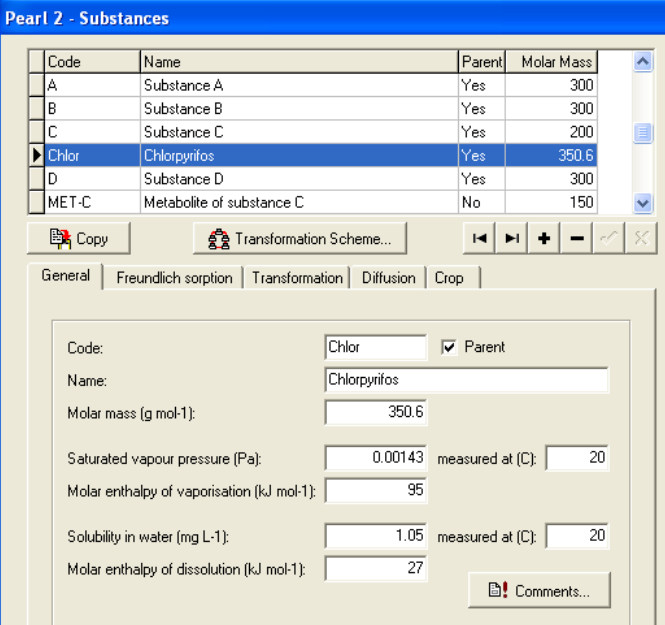
What if you choose the wrong model?



test of MACRO and PEARL for bentazone leaching from drain pipes on Dutch heavy clay soil: preferential flow model needed for description of early breakthrough

3. Definitions: source/calculation kernel, GUI, database

- Source/calculation kernel: calculations written in programming language, e.g. Fortran
- Data base: contains information on e.g. meteo, soils, pesticide properties
- Graphical User Interface (GUI): to make use simple (user friendly)



The screenshot shows the 'Pearl 2 - Substances' window. At the top, there is a table listing substances with columns for Code, Name, Parent, and Molar Mass. The 'Chlor' substance is selected. Below the table, there are buttons for 'Copy' and 'Transformation Scheme...'. A tabbed interface below shows the 'General' tab selected, displaying a form for the selected substance 'Chlorpyrifos'. The form includes fields for Code, Name, Molar mass, Saturated vapour pressure, Molar enthalpy of vaporisation, Solubility in water, and Molar enthalpy of dissolution, each with a value and a 'measured at (C):' field. A 'Comments...' button is also present.

Code	Name	Parent	Molar Mass
A	Substance A	Yes	300
B	Substance B	Yes	300
C	Substance C	Yes	200
▶ Chlor	Chlorpyrifos	Yes	350.6
D	Substance D	Yes	300
MET-C	Metabolite of substance C	No	150

Code: Chlor Parent

Name: Chlorpyrifos

Molar mass (g mol⁻¹): 350.6

Saturated vapour pressure (Pa): 0.00143 measured at (C): 20

Molar enthalpy of vaporisation (kJ mol⁻¹): 95

Solubility in water (mg L⁻¹): 1.05 measured at (C): 20

Molar enthalpy of dissolution (kJ mol⁻¹): 27

Comments...

Definitions: Validation of models, e.g. leaching models

- Validation status
 - Boesten (2000): in general pesticide leaching models are reliable to assess the leaching of the bulk of the dose (above 1% of dose)
 - EU drinking water limit = $0.1 \mu\text{g/L}$ \rightarrow 0.1 % of dose of 1kg/ha (assuming 100 mm/year percolation)
 - Validation status of models at this level of leaching is still low!
 - Boesten (2000). From laboratory to field: uses limitations of pesticide behaviour model for the soil/plant system. Weed research, 40:123-138