Refinements to the MARTHE model to enable the simulation of the fate of agricultural contaminants from the soil surface to and in groundwater

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Outline of the presentation

- **Presentation initially given at the COST workshop in May 2004 in Rome**
- **Work undertaken as part of the FP5 project PEGASE (Pesticides in European Groundwaters)**
- **Provide you with an overview of:**
  - the MARTHE model
  - the modifications made to the model to enable the simulation of the **fate of pesticides from the soil surface to and in groundwater** (i.e. soil, unsaturated and saturated zones)

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MARTHE

Modelling Aquifers with an irregular Rectangular grid, Transport, Hydrodynamics and Exchanges

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A bit of history

- **Code initially developed by BRGM in the mid 1980s**
- **Code developper: Dominique Thiéry**
- **Initially developed to simulate water flow in the saturated zone in 3D**
- **Later adapted to simulate flow in the unsaturated zone + solute transport and fate**
- **Regular updates to include the latest developments in process description and numerical techniques**

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Main characteristics

- **Finite volumes approach**
- **Solving of the Richards' equation with a range of retention and hydraulic conductivity laws (VG,B&C, Brusaert, Gardner, homographic, power law)**
- **Three techniques for simulating advective, diffusive and dispersive transport (Donor cell, Total Variation Diminishing, Method of Characteristics)**
- **All calculations for energy, temperature, mass and water fluxes are fully integrated**
- **Water, reactive and non-reactive contaminants, oil, gas**
- **Hor. Discretization: (ir)regular rectangular grid**
- **Vert. Discretization: 3D or complex multilayer system**
- **Integrates processors and tools: spatial handling of input and output data, contouring, sensitivity analysis, inverse modelling**
- **Can be coupled to other models (e.g. geochemical)**

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Applications

- **MARTHE has been applied to >200 aquifer systems in France and overseas**
  - management of GW resources (e.g. water balance assessment, impact of abstractions)
  - civil engineering and mining work
  - environmental assessments (point and diffuse sources)
- **Spatial scale: from cells of a few mm to GW multilayer systems of 150,000 km²**
- **Temporal scale: from a few seconds to 15,000 years**

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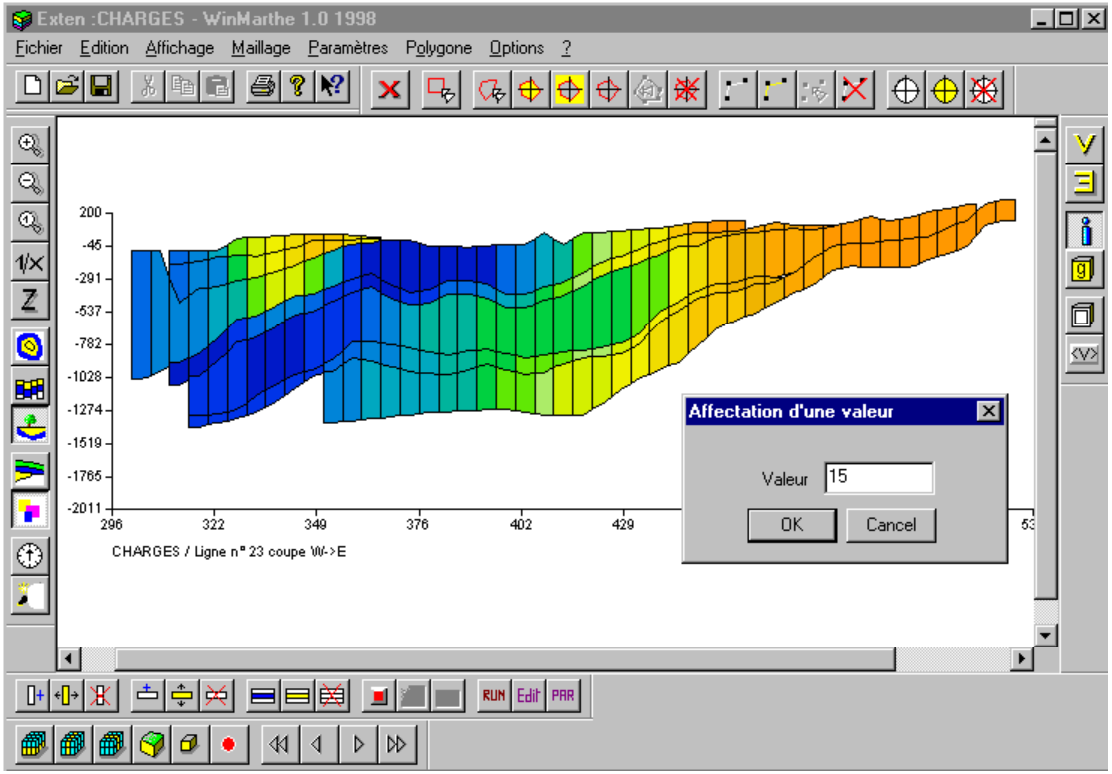
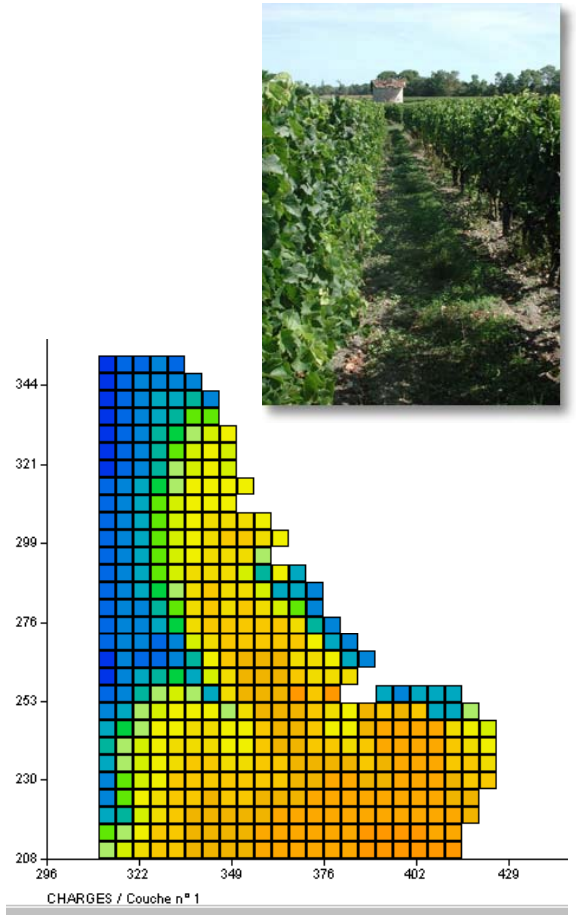
Model interface



Vertical cross section of hydraulic heads in the Bordeaux region



Horizontal cross section

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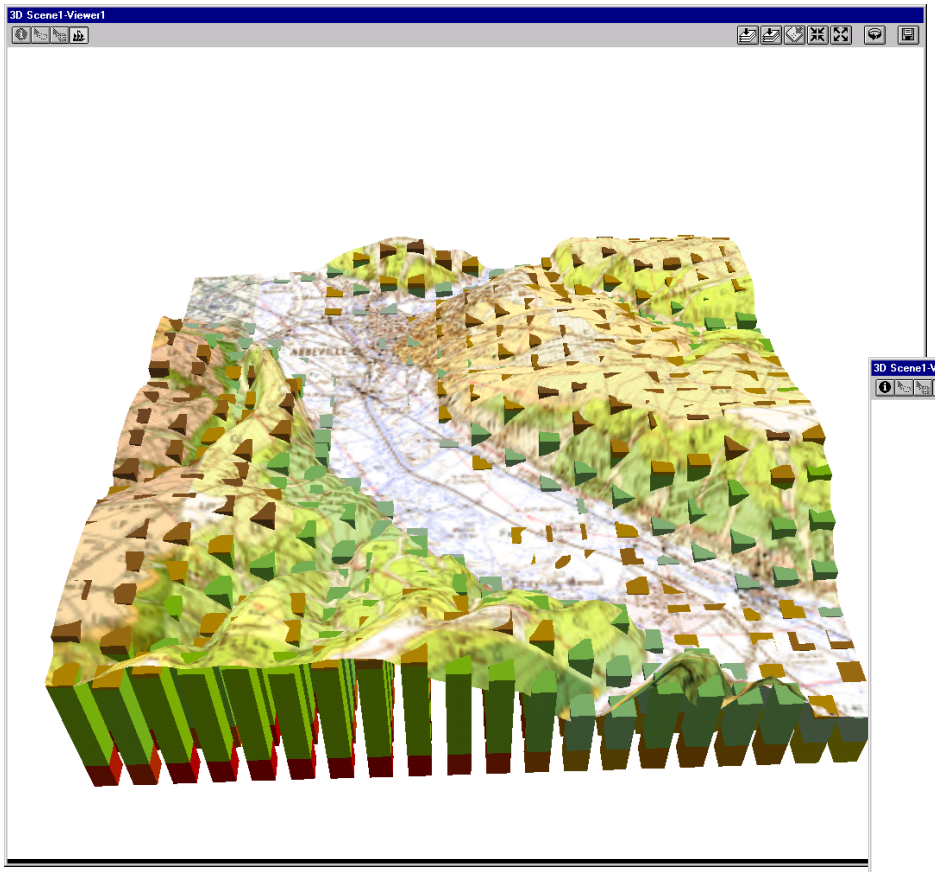
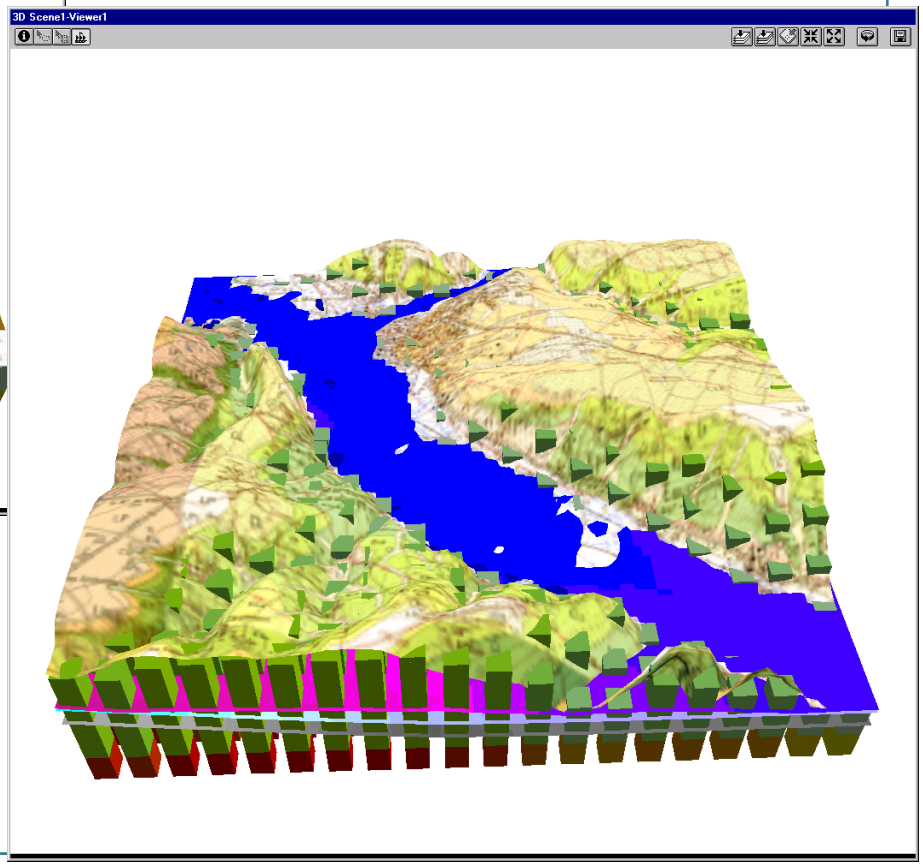
Example of application





Contribution of GW to floods in the Somme valley (2001)

Modifications of MARTHE to simulate pesticide fate

Work funded by the EU
PEGASE European project (1999-2003)
http://www.brgm.fr/pegase

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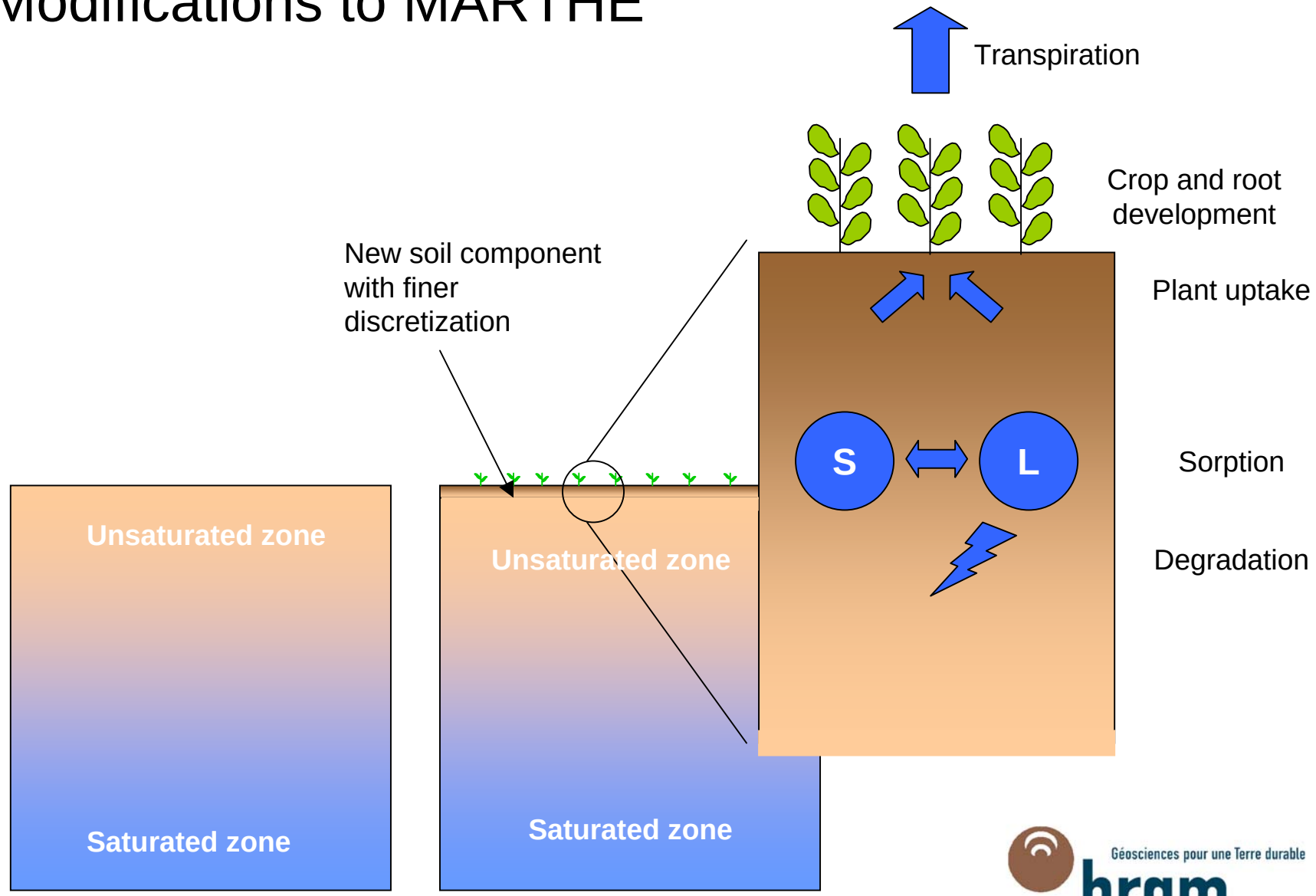
Modifications to MARTHE



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Process description

- **Cropping**
  - Crop and root development (root depth and density: MACRO, AGRIFLUX)
  - Transpiration according to LEACHP, AGRIFLUX and MACRO schemes
  - Hydric stress according to SWAP and MACRO
  - Crop uptake of water and pesticides

- **Sorption:**
  - Freundlich + Langmuir
  - Mobile-immobile concept

- **Degradation:**
  - 2 degradation schemes: linear + one generation of daughter products
  - First-order kinetics
  - Effect of temperature and humidity on degradation: 5 different schemes (LEACHP, AGRIFLUX, MACRO, WAVE, PELMO)

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Concept of versatility

- **Do a thorough review of the various approaches used to simulate a given process (literature, models)**
- **Select a range of approaches and include them in the model**

- **Benefits**
  - comparison of approaches used in different models
  - combination of approaches used in different models
  - the model user is in control
  - analysis of the uncertainty resulting from model selection

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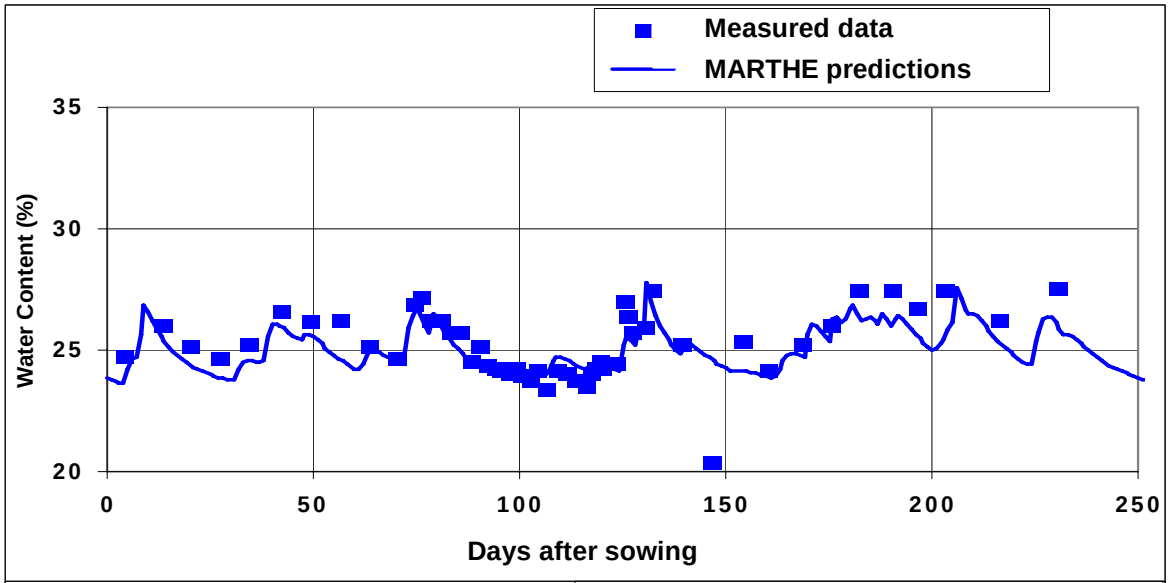
Model verification

- **Validation process to build confidence in the new version of the model**
- **Three steps**
  - Step 1: individual subroutines
  - Step 2: combination of subroutines
  - Step 3: whole environmental system

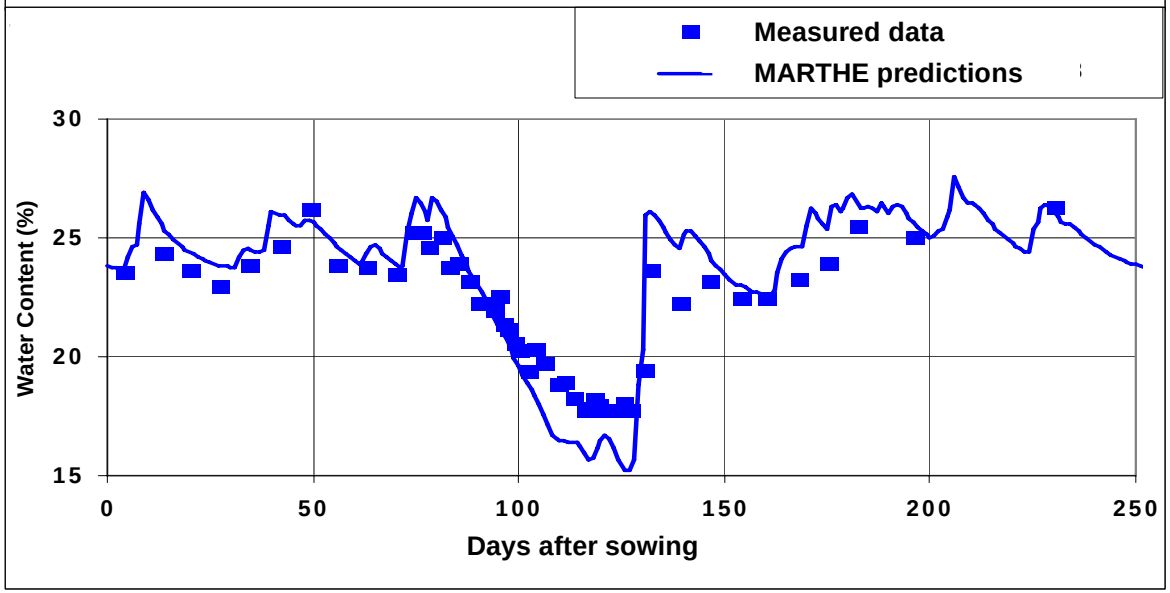
	Field data	Analytical solutions
Crop and root development	La Côte Saint André (WC on bare and maize plots)	-
Sorption	-	Langmuir: Zheng et al., 1998 Freundlich: Huang et al., 1998
Degradation	-	Cho (1971) & van Gen. (1985) $NH_4^+ \rightarrow NO_2 \rightarrow NO_3^-$

Model verification - transpiration and water balance

Bare soil

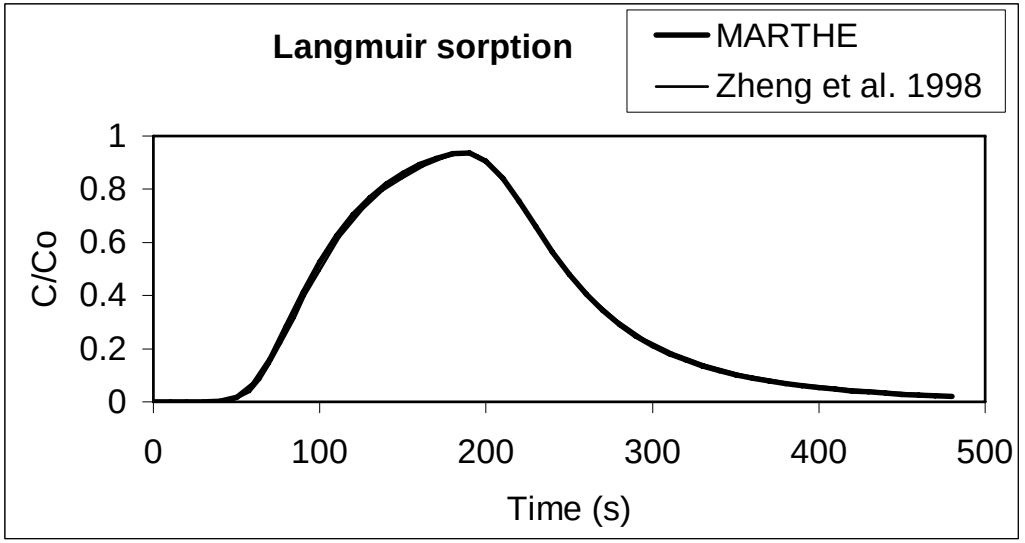


Maize

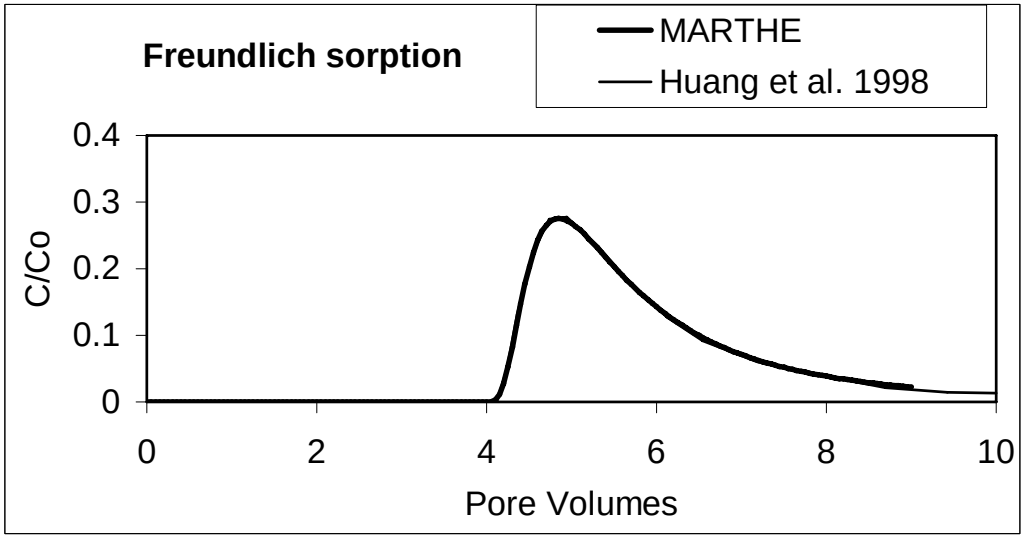


Model verification - sorption

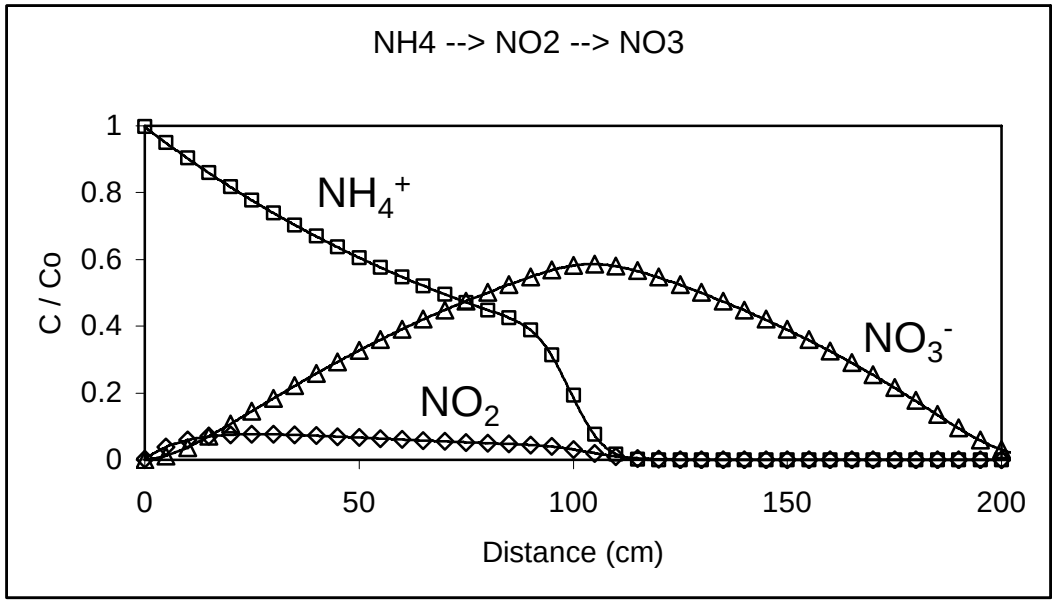
Langmuir



Freundlich



Model verification - degradation



Lines: MARTHE
Symbols: Analytical solutions

Transport of NH_4^+, NO_2 and NO_3^- in a horizontal column

Cho (1971) & van Gen. (1985)

Potentialities offered by MARTHE in the field of pesticide fate modelling

> **Complement existing pesticide fate models based on its own specificities:**
  - 1- to 3-D model (2D applications)
  - Range of scales
  - Transport and fate in soil, unsaturated and saturated zones (true continuum)
  - Comparison of models and modelling approaches (uncertainty aspects)

> **Higher tier applications**
  - below 1-m depth, dealing with real systems
  - combination of post-registration monitoring and modelling
  - fate in groundwater systems
  - e.g. investigate the reasons for detection of significant pesticide concentrations in groundwater at specific locations

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Future activities with MARTHE

- **Encourage collaborative work with the model**

- **Further evaluate MARTHE against:**
  - Field leaching and lysimeter data (1-m depth)
  - Catchment scale pesticide data (Soil - Unsaturated zone - Saturated zone continuum)

- **Further improve the capabilities of the model by allowing the simulation of:**
  - more complex degradation schemes
  - preferential flow based a range of 1D- and 2D-approaches (work being undertaken within the FP6 project AquaTerra)

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