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Department of Applied Mathematics, Biometrics and Process Control

Harmonising chemical fate and basic water quality modelling at the catchment scale

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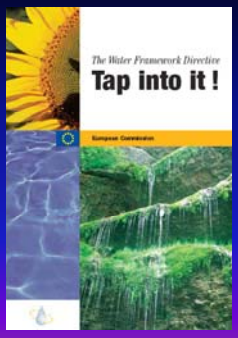
Water Framework Directive (WFD)

- WFD = European policy basis for **river basin management plans**
- WFD requires **integration and collaboration** of different domains and various stakeholders.
- Increasing need for guided use and supporting methodologies of **harmonised** high quality computer based tools



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Issue

	Chemical fate modelling	Basic water quality modelling
• Type pollutant	Organic contaminants	Organic loads and nutrients
• Communities	SETAC	IWA, EGU
• Model complexity	Steady-state	Steady-state & dynamic
• Model performance	Low-moderate (factor 5-100)	Moderate-high (factor <10)

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Goal

- Integrated approach beneficial for WFD
- Solution: INTEGRATION ON

"LOGISTIC" LEVEL

– Harmoni-CA as a forum for harmonising ICT tools for integrated river basin management

TECHNICAL LEVEL

– present – conceptually and with examples – integrated chemical fate and water quality modelling

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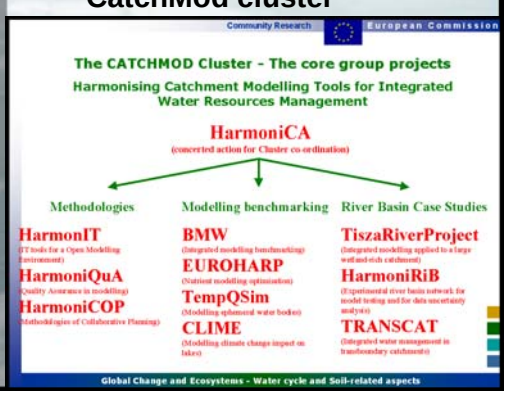
What is Harmoni-CA (1)?

- Large-scale EU concerted action
- Does not carry out a research, but synthesises available knowledge
- Typical actions are meetings and workshops, leading to synthesis reports and guidances
- http://www.harmoni-ca.info

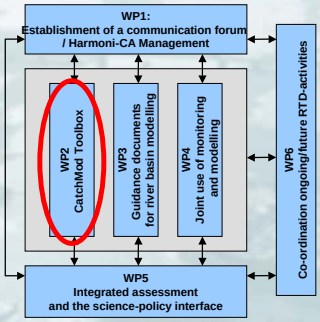
What is Harmoni-CA (2)?

CatchMod cluster



What is Harmoni-CA (3)?

Harmoni-CA work packages



CatchMod Toolbox (1)

Through a website, provide easy and guided access/links to:

- open, flexible, scientific sound toolbox for present and future integrated, harmonised ICT-tools.
- benchmarking reports
- tools selection tool
- resources, training material, demo case studies, protocols , IPR
- Web-based simulations

CatchMod Toolbox (2)

- This guides the user to the tools based on the issue at hand, the characteristics of the river basin, the data availability etc.
- Call for toolboxes
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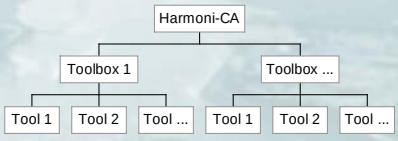
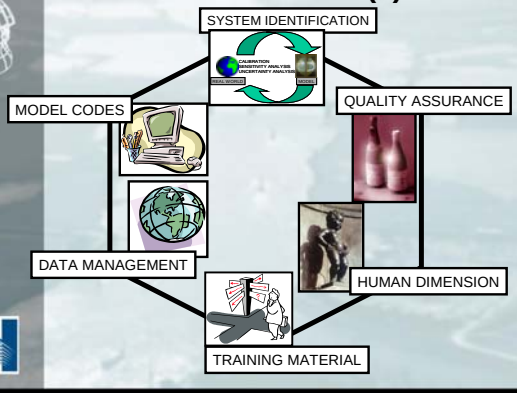


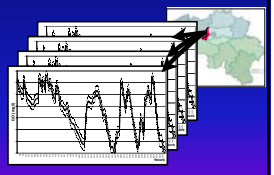
CatchMod Toolbox (3)



Technical integration: model complexity

Chemical fate modelling	Basic water quality modelling
steady-state	steady-state/dynamic

LAS concentrations (PECs)



Dissolved oxygen concentrations

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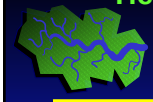
"Tiered" integrated approach



	Chemical fate modelling	Basic water quality modelling
• Steady-state Conc (avg or worst)	E-USES,…	QUAL2E,…
• Probabilistic Conc. distribution	Monte Carlo in GREAT-ER, …	SIMCAT,…
• Dynamic Time-series	*Under development*	RWQM, MIKESHE,ISIS, SWAT,…

(Deksissa, 2004)

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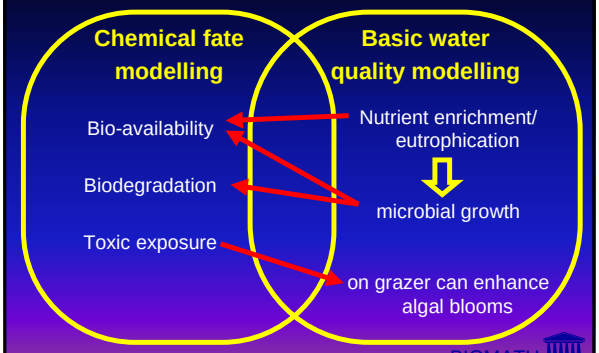
Technical integration: example interactions



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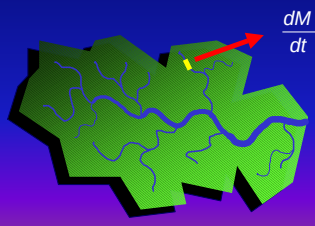
Technical integration

Main principle in catchment-based models:

- Mass balance



$$\frac{dM}{dt} = L_{in} - L_{out} \pm reactions$$

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Technical integration

- Reactions

Chemical fate modelling

- Aerobic biodegradation of Generic organic compounds (S_{GC})
  - Monod

$$\frac{dS_{GC}}{dt} = -k_{h,T} \frac{S_{GC}}{K_{GC} + S_{GC}} \frac{S_{O2}}{K_{O2} + S_{O2}} X_H$$

  - First order

$$\frac{dS_{GC}}{dt} = -k_{h,T} S_{GC} \frac{S_{O2}}{K_{O2} + S_{O2}} X_H$$

Basic water quality modelling (e.g. RWQM No.1)

- Biomass growth

$$\frac{dX_H}{dt} = k_{grow,T} \frac{S_N}{K_N + S_N} \frac{S_P}{K_P + S_P} \cdot \frac{S_S}{K_S + S_S} \frac{S_{O2}}{K_{O2} + S_{O2}} X_H$$

$$\frac{dS_{O2}}{dt} = \ldots$$

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Conclusions

- In view of WFD, integration of chemical fate & basic water quality modelling (incl. their interaction) would be beneficial.
- Harmoni-CA provides a forum
  http://www.harmoni-ca.info

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