Sveriges lantbruksuniversitet
Swedish University of Agricultural Sciences

MACRO-based modelling tools
- Recent development and future plans

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Two parts:

- MACRO-DB: A tool for risk assessments for permits in drinking water abstraction zones
- Modelling soil freezing

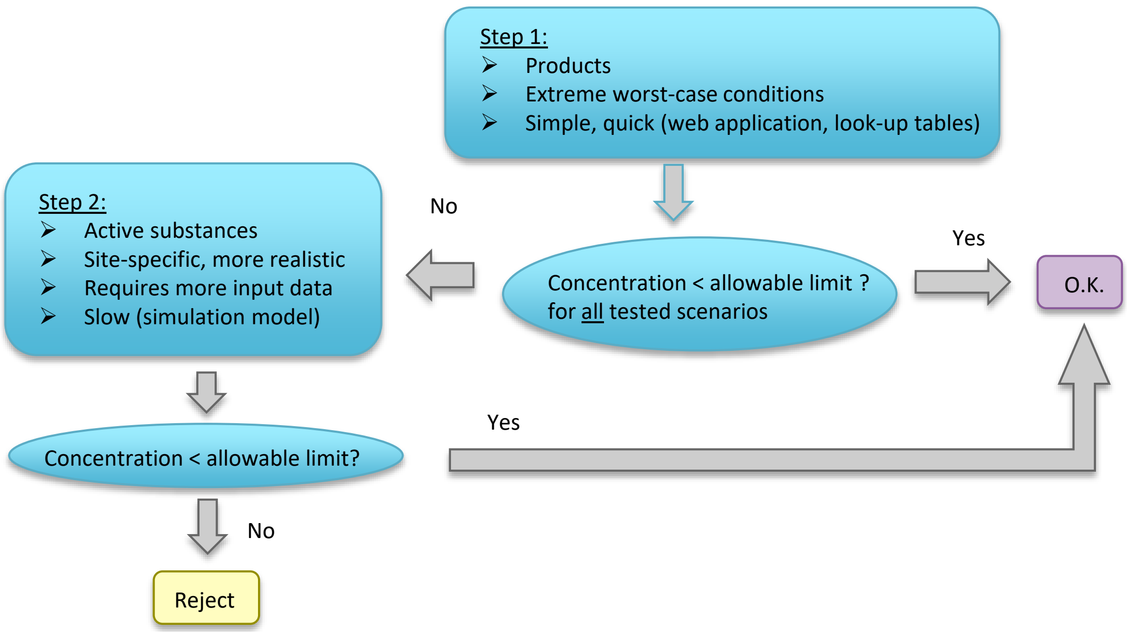
MACRO-tools

Tool	Use	End-users
MACRO in FOCUS	Registration (nationally and EU)	National authorities (e.g. Swedish Chemicals Agency), EFSA, industry
+MACRO-DB	Application permits in drinking water protection areas	Local authorities, landowners, consultants, advisors
+MACRO-SE	Support for risk reduction/mitigation (EU Water Framework Directive), targeted environmental monitoring	Regional water authorities (EPA, SGU)

+Development of MACRO-DB/SE is supported by CKB and HaV, the Swedish Agency for Marine and Water Management

MACRO-DB: risk assessment for permits in drinking water abstraction zones

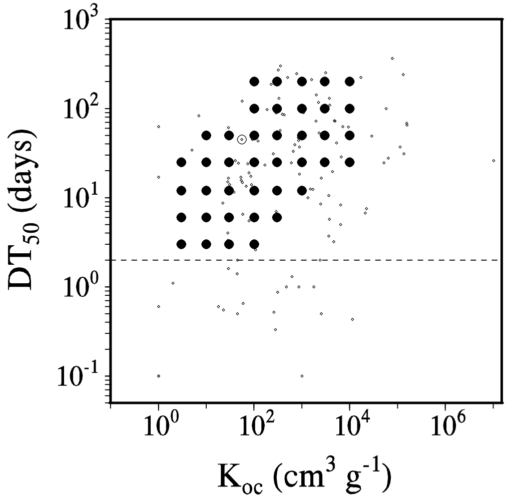
A two-step procedure



MACRO-DB: risk assessment for permits in drinking water abstraction zones

Step 1

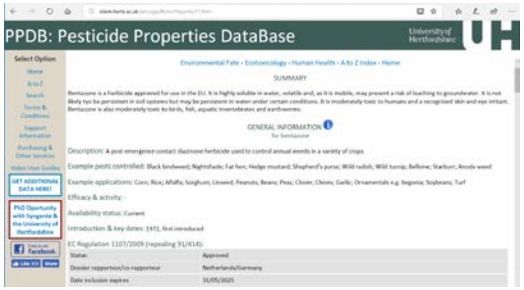
- Web-application (immediate answers)
- Simple input data
  - Product, dose, application timing and climate zone
  - How often is the product applied? (i.e. every year, every other year, every third etc.),
  - Proportion of arable land in catchment area
- Already run 'worst-case' simulations
  - Eleven common soil types (hydrology/texture):
  - 5th percentile SOM in topsoil
  - 95th percentile for texture (sandy sand soils, clayey clay soils)
  - 51 hypothetical compounds
- Model
  - Linear adsorption isotherm

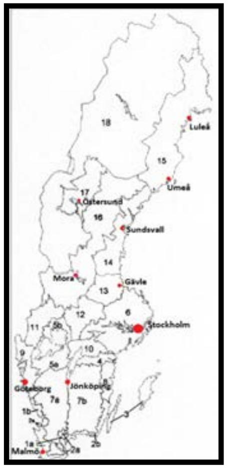


MACRO-DB: risk assessment for permits in drinking water abstraction zones

Step 2

Applications
Crop, compound properties (PPDB), dose, timing (2 week periods), method



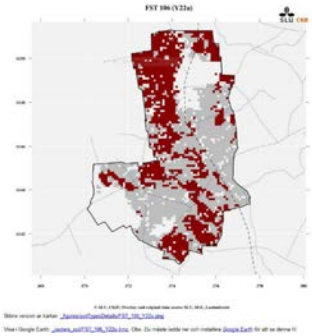


Climate data
Daily data for 26 years
Climate zones in Sweden

Pedotransfer rules and functions (FOOTPRINT)

Parent material
Quaternary geology

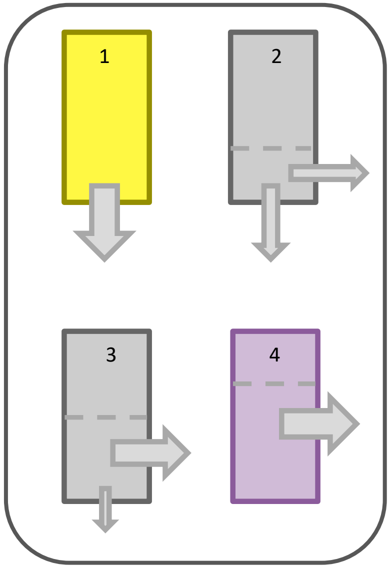
Soil properties
Texture, SOM



Soil hydrological classification

Quaternary geology	**Subsoil texture**	**Hydrological class**	
		Drained	**Undrained**
Coarse esker materials		-	1
Sedimentary rocks		-	1
Moraine (till)	Coarse	-	2
	medium, medium-fine	3	2
	Fine	3	-
Rock		-	3
Coarse silt/fine sand, sand or gravel		4	2
Clay/silt		4	2
Organic soil (peat)		4	-
Alluvium/outwash		4	-

Red = recharge area
Blue = both recharge and discharge area
Grey = discharge area



Development plans (feedback welcome!)

- The current version is time-consuming for farmers and authorities to use and also difficult (expensive) for us (CKB) to maintain
- *HaV* are supporting a recently-started project to develop meta-models to replace the current two-step procedure
  - Web application
  - Meta-model(s) based on ca. 900,000 simulations
    - Ca. 40 major/sensitive soil-hydrological types,
    - 16 climate zones
    - 3 generic crop types
    - 3 application timings (spring, summer, autumn)
    - Ca. 120 hypothetical pesticides (3 Freundlich exponents, 50 combinations of DT_{50}/K_{oc})
  - Best statistical method? We will test CART (classification and regression trees)

Modelling soil freezing

Background

- Significant losses of pesticides may occur when the soil is partly frozen (Riise et al., 2004; Ulén et al., 2013)
- Soil freezing is not accounted for in risk assessments for pesticides
- As far as we know there are no models that account for both freezing and preferential flow and transport

Riise, G., H. Lundekvam, Q. L. Wu, L. E. Haugen and J. Mulder (2004). "Loss of Pesticides from Agricultural Fields in SE Norway – Runoff Through Surface and Drainage Water." Environmental Geochemistry and Health **26(2): 269-276.**

Ulen, B. M., M. Larsbo, J. K. Kreuger and A. Svanback (2013). "Spatial variation in herbicide leaching from a marine clay soil via subsurface drains." Pest Management Science **70(3): 405-414.**

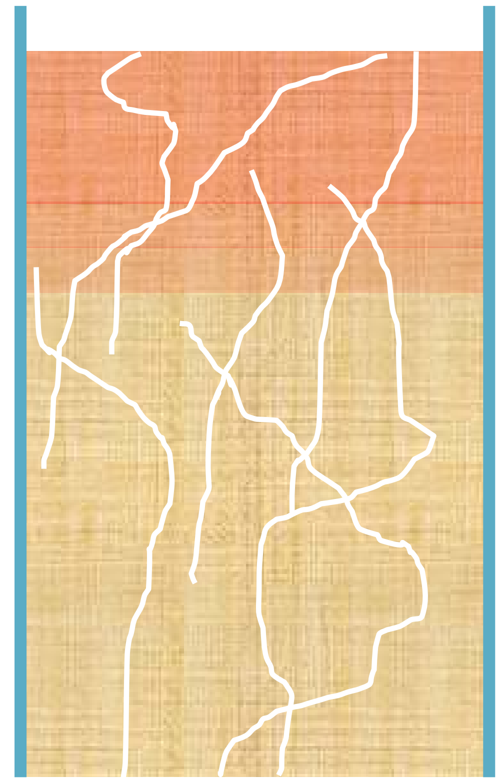
Schematic illustration of solute transport in frozen soil

Schematic illustration of solute transport in frozen soil

Frozen

Unfrozen

Schematic illustration of solute transport in frozen soil



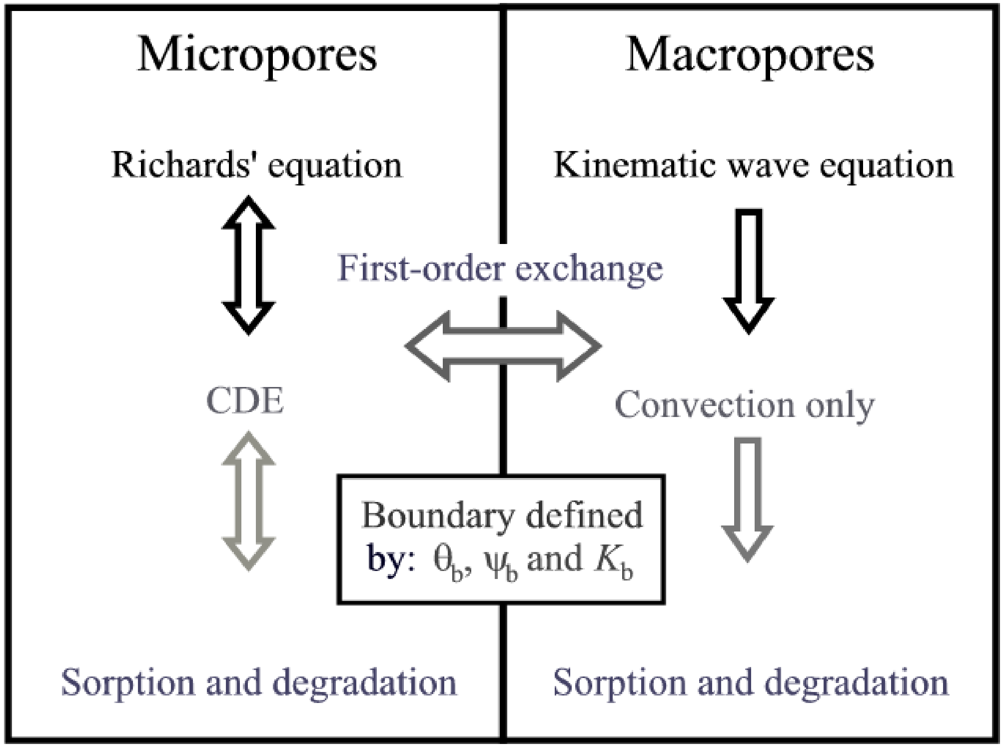
Frozen **Unfrozen**

Objective

Develop and evaluate a dual-permeability approach for simulating water flow (and solute transport) in soil under freezing and thawing conditions.

Frozen **Unfrozen**

The MACRO model



- Dual-permeability approach for water flow and solute transport
- Single domain for soil temperatures
- Freezing and thawing not simulated

Modelling approach freezing

Micropore domain

- Large (water-filled) pores freeze first

→

- Large effect on hydraulic conductivities
- "Freezing = drying"

Macropore domain

- No effects of capillary pressure on freezing
- Smallest (water-filled) macropores freeze first

Modelling approach freezing

Micropore domain

Heat flow equation (conduction and convection)

Generalized Clapeyron equation

Richard's equation

Macropore domain

- Heat convection only
- Macropores will only freeze through exchange with the micropore domain

Hansson, K., J. Šimůnek, M. Mizoguchi, L.-C. Lundin and M. T. van Genuchten (2004). "Water Flow and Heat Transport in Frozen Soil." Vadose Zone J. **3(2): 693-704.**

Stähli, M., P. E. Jansson and L. C. Lundin (1996). "Preferential water flow in a frozen soil - A two-domain model approach." Hydrological Processes **10(10): 1305-1316.**

Model evaluation

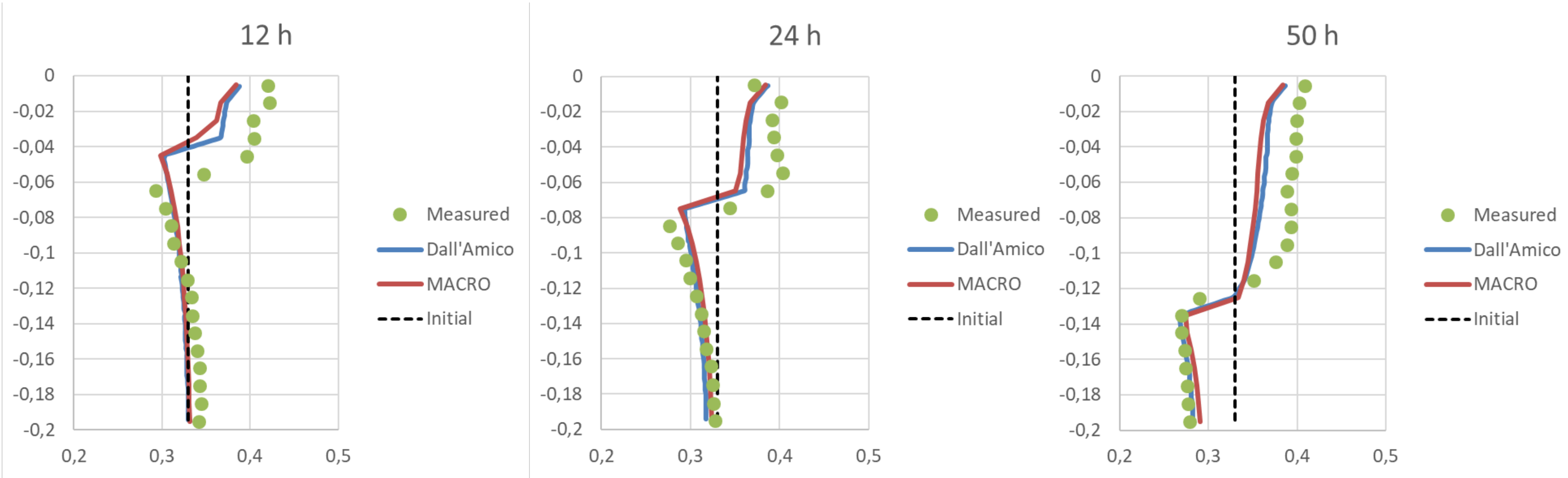
Redistribution of water – freezing from the soil surface

<u>Only soil matrix</u>

Initial conditions: Water content = 0.33; Soil temperature = 6.7 °C

Top boundary condition: Temperature = -6 ^{o}C; No water flow

Bottom boundary: No flow

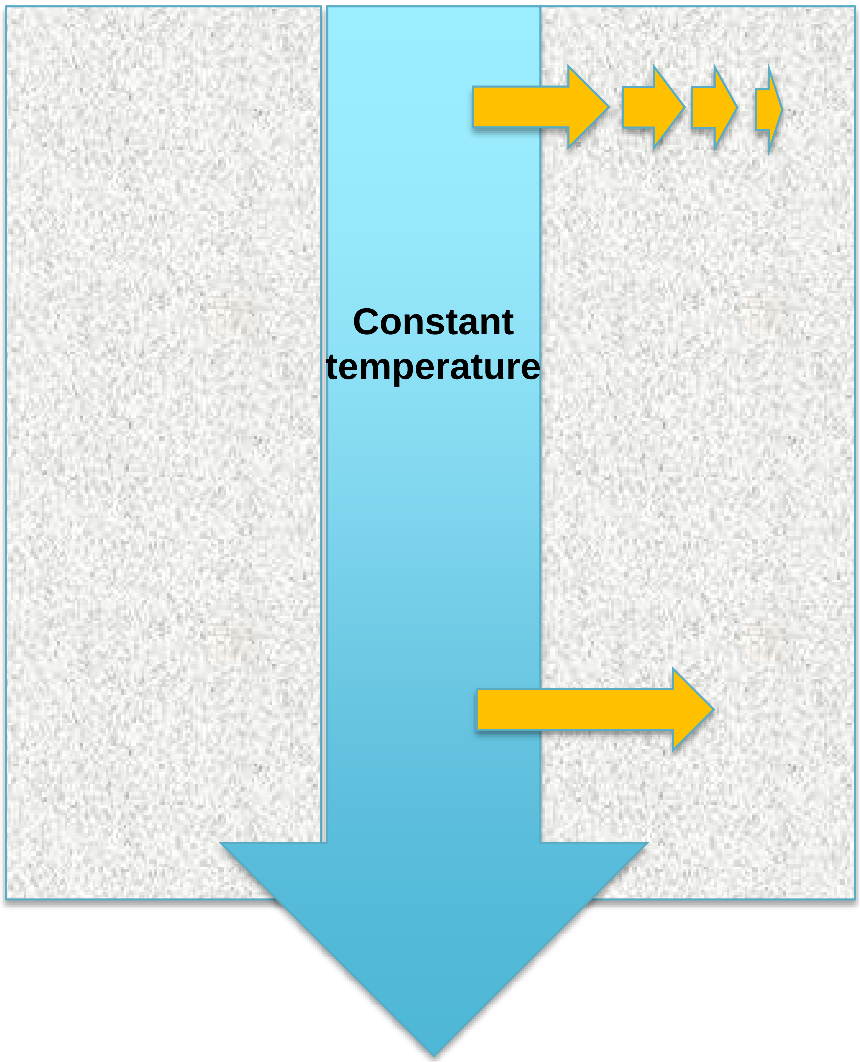


Mizoguchi, M. 1990, Water, heat and salt transport in freezing soils. PhD thesis (In Japanese), University of Tokyo.

Dall'Amico, M., S. Endrizzi, S. Gruber and R. Rigon (2011). "A robust and energy-conserving model of freezing variably-saturated soil." <u>Cryosphere</u> **<u>5(2): 469-484.</u>**

Model evaluation

Energy exchange between pore domains



Heat conduction equation

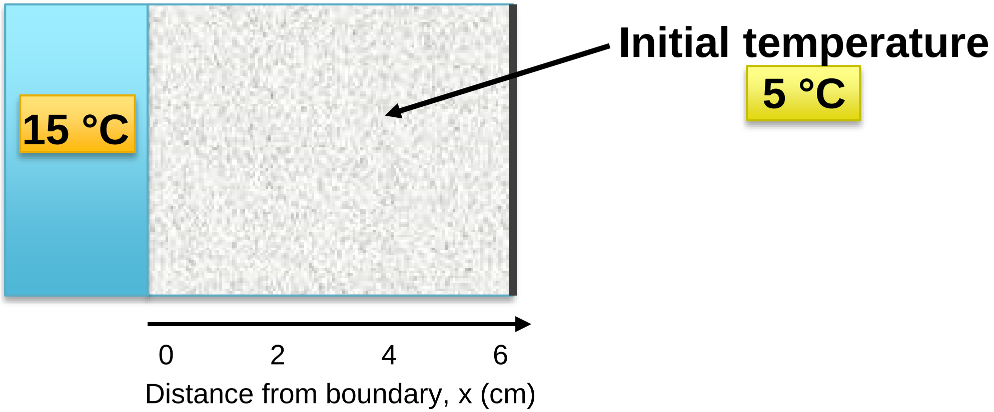
$$\frac{\partial C_v T}{\partial t} = \frac{\partial}{\partial x}\left(k_h \frac{\partial T}{\partial x}\right)$$

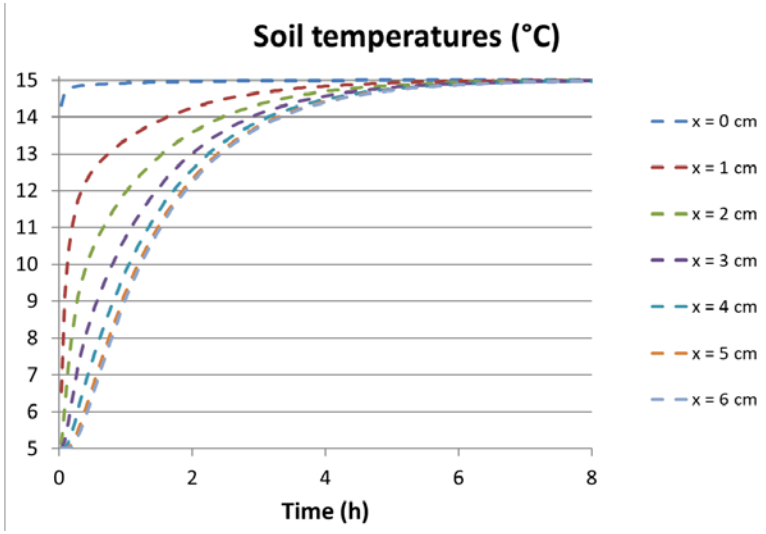
First-order approximation to the heat conduction equation

$$\frac{\partial C_v T}{\partial t} = \frac{G_f k_h S_{mac,tot}}{d^2}(T_{mic-} T_{mac})$$

Model evaluation

Energy exchange between pore domains





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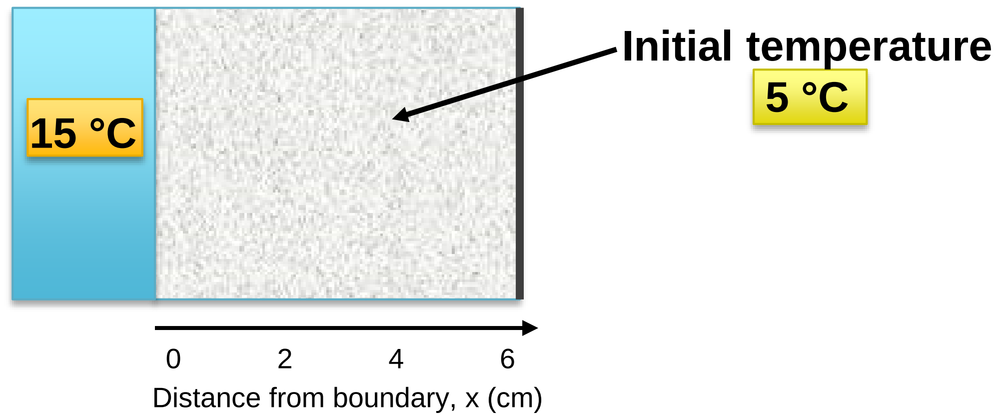
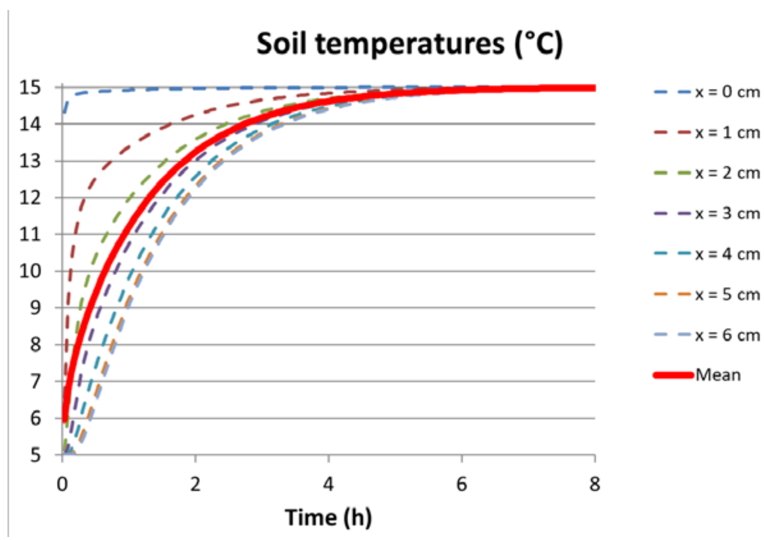
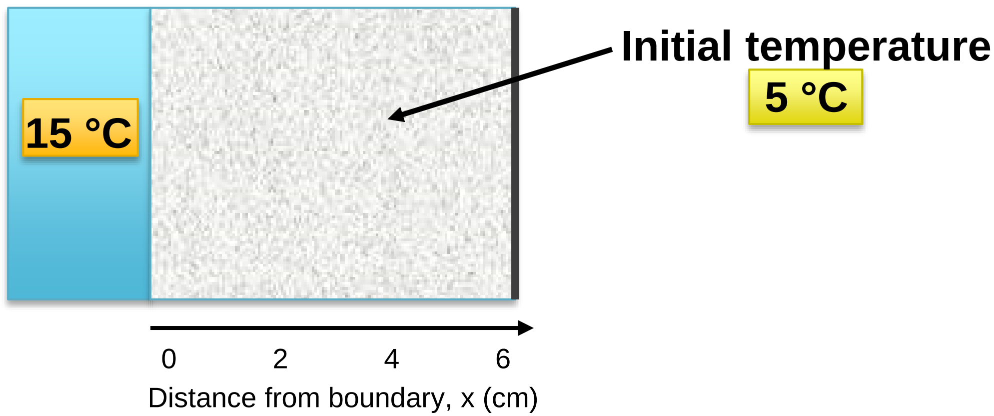
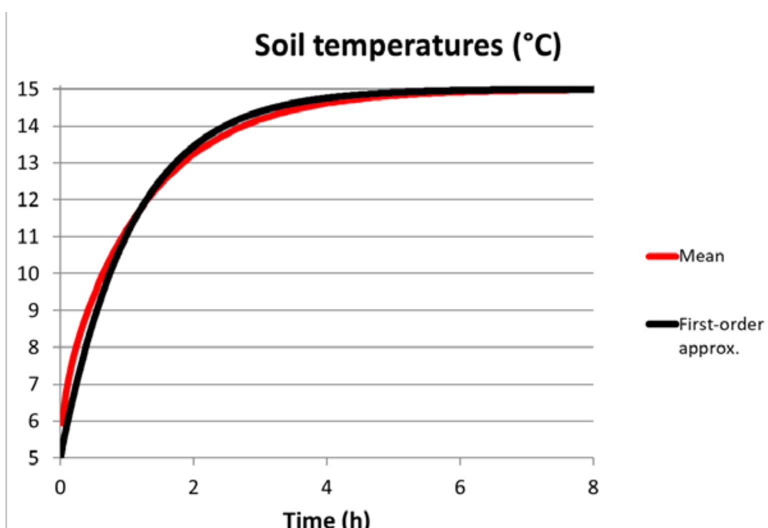




Model evaluation

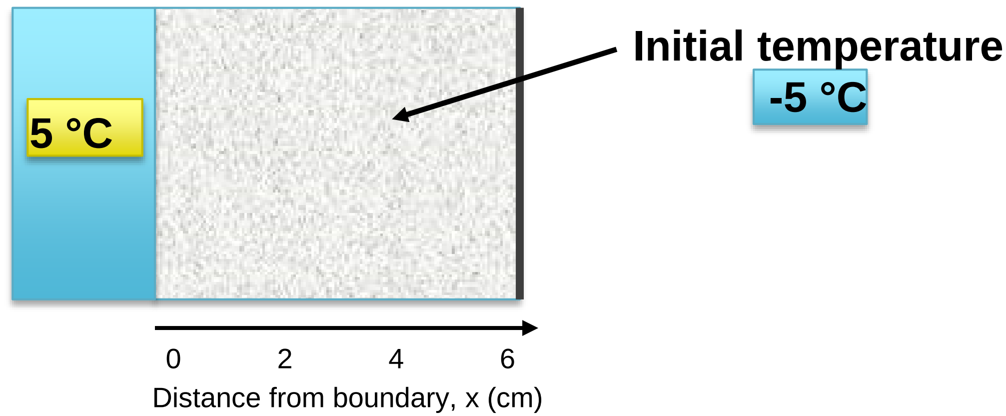
Energy exchange between pore domains

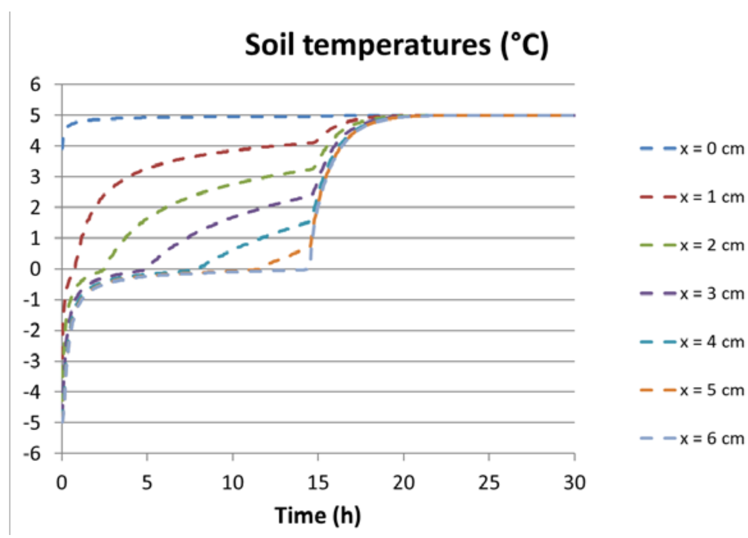




Model evaluation

Energy exchange between pore domains





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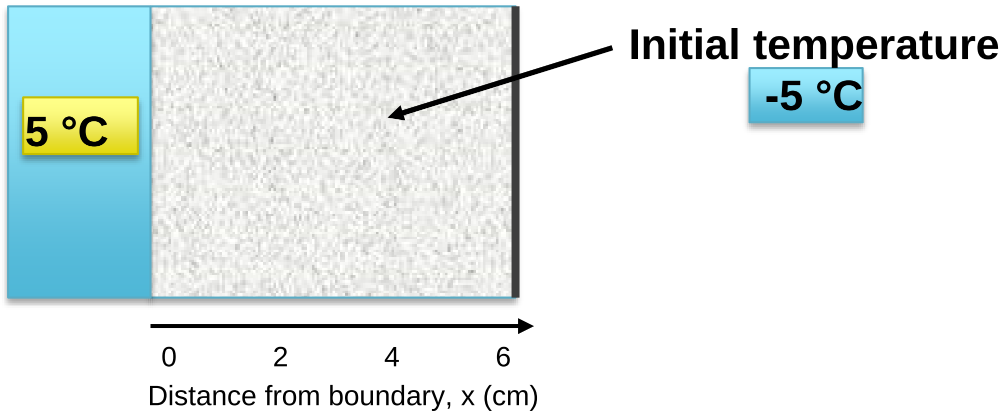
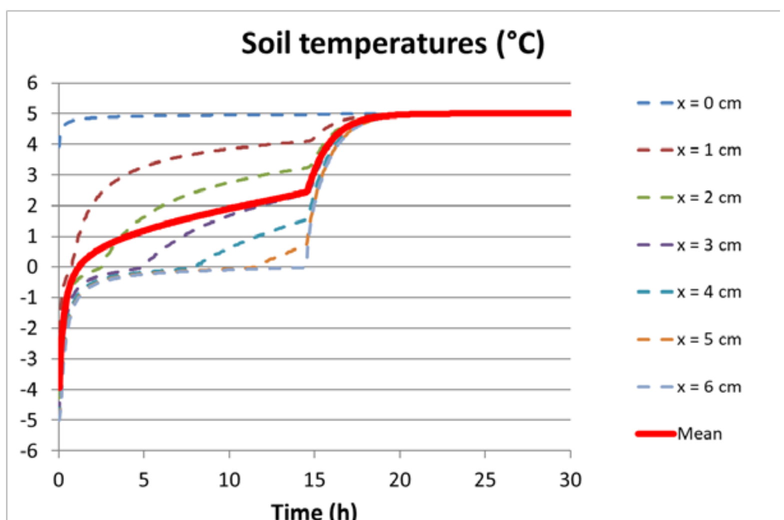
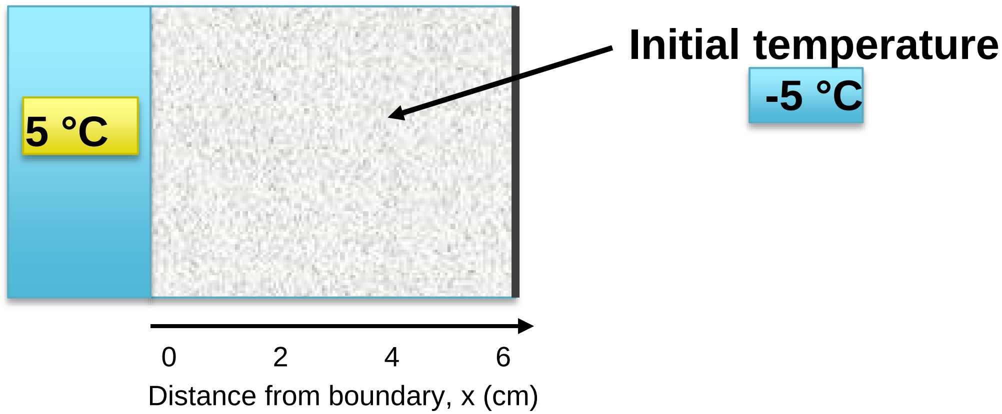
Energy exchange between pore domains

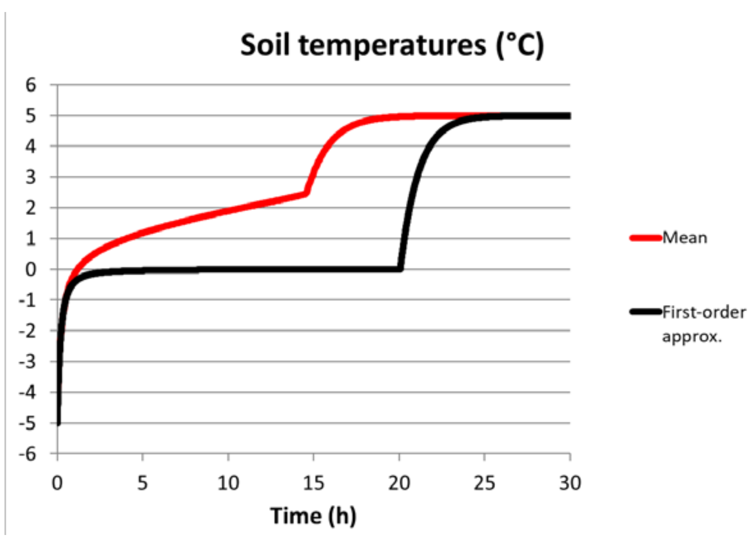




Model evaluation

Energy exchange between pore domains



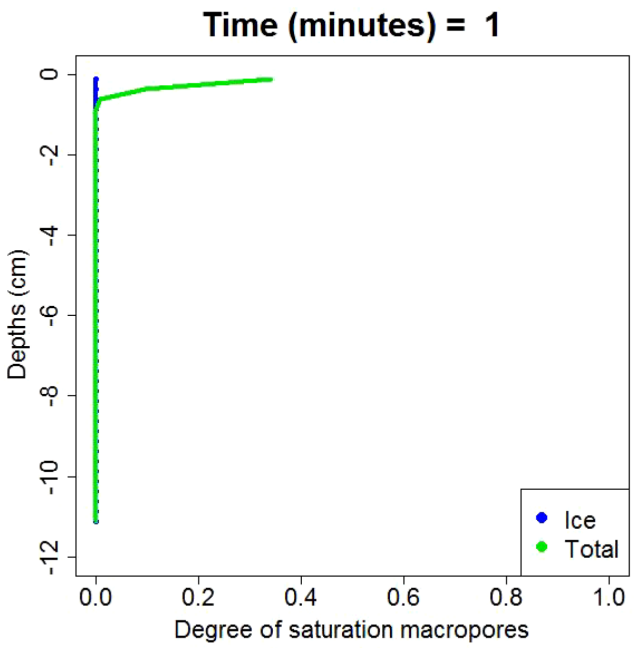


Model evaluation

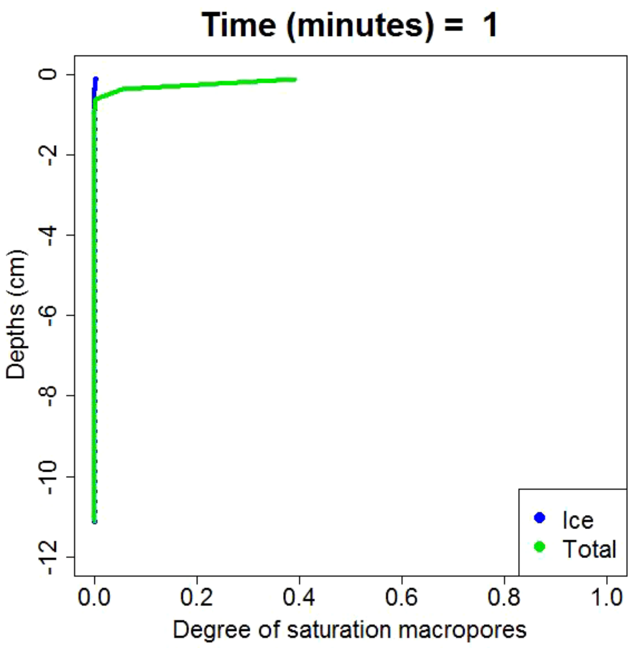
Water flow in macropores

Surface boundary condition:
6 min irrigation every 30 min
Temperature of water 1 °C

Initial condition:
Air-filled macropores
Saturated matrix at **1 °C**



Initial condition:
Air-filled macropores
Saturated matrix at **-2 °C**

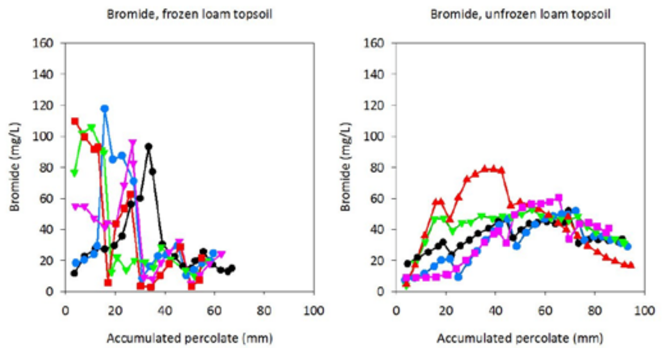


Conclusions…

- The model results are in agreement with the limited available data
- Inclusion of freezing effects in risk assessments for pesticides lies in the future

…and future plans

- “Validation” of the macropore freezing/water flow model
- Connect water flow and solute transport
- Evaluation of the complete model using data from column experiments



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Thanks for listening!