

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

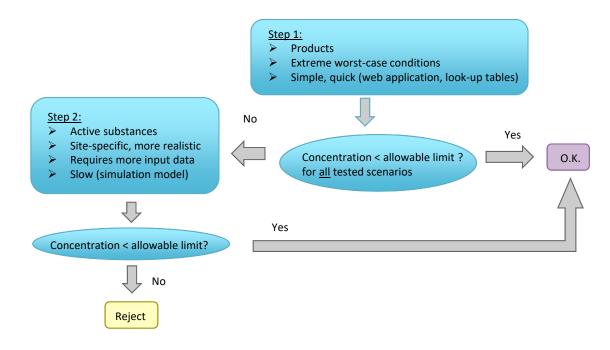
ΤοοΙ	Use	End-users
MACRO in FOCUS	Registration (nationally and EU)	National authorities (e.g. Swedish Chemicals Agency), EFSA, industry
⁺ MACRO-DB	Application permits in drinking water protection areas	Local authorities, landowners, consultants, advisors
*MACRO-SE	Support for risk reduction/mitigation (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

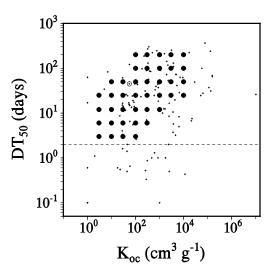




MACRO-DB: risk assessment for permits in drinking water abstraction zones

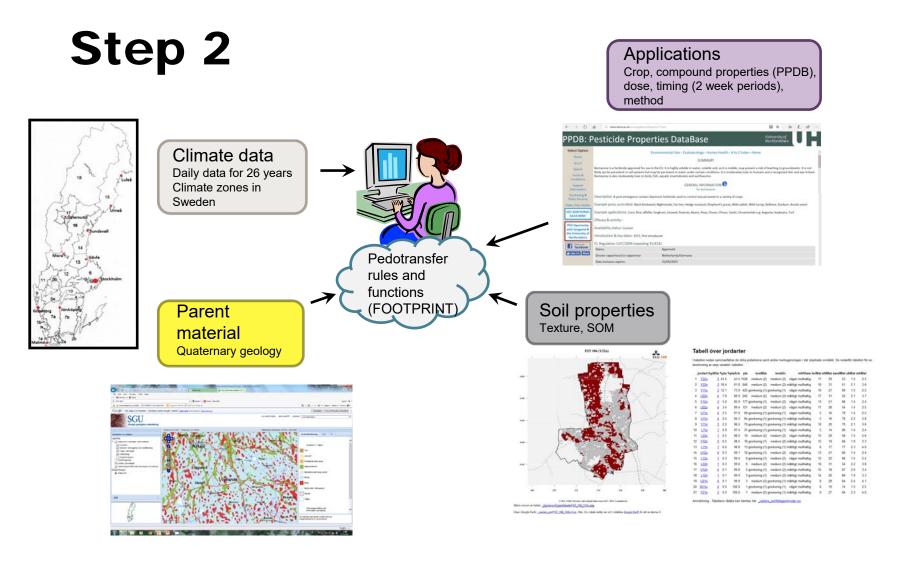
Step 1

- 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

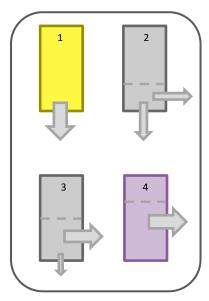




Soil hydrological classification

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 $\text{DT}_{50}/\text{K}_{\text{oc}})$
 - Best statistical method? We will test CART (classification and regression trees)



Modelling soil freezing



Background



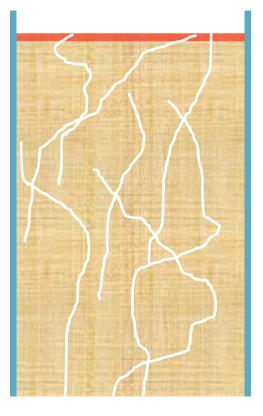
- Significant losses of pesticides may occur when the soil is partly frozen (Riise et al., 2004; Ulén et al., 2013)
- Soil freezing is not accounted for in risk assessments for pesticides
- As far as we know there are no models that account for both freezing and preferential flow and transport

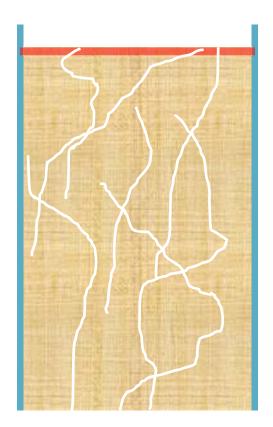
Riise, G., H. Lundekvam, Q. L. Wu, L. E. Haugen and J. Mulder (2004). "Loss of Pesticides from Agricultural Fields in SE Norway – Runoff Through Surface and Drainage Water." <u>Environmental Geochemistry and Health **26(2): 269-276.**</u>

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." <u>Pest Management Science **70(3): 405-414.**</u>



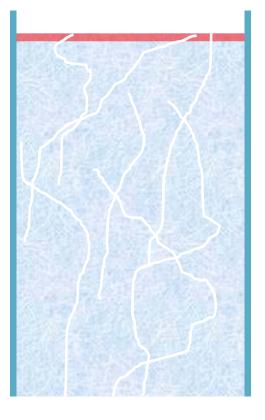
Schematic illustration of solute transport in frozen soil







Schematic illustration of solute transport in frozen soil



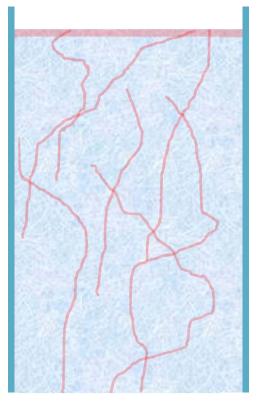


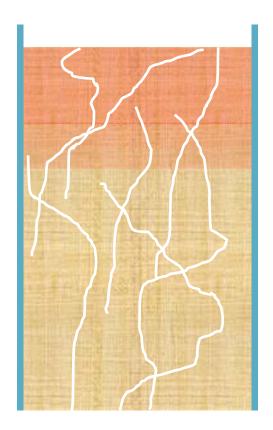
Frozen

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.



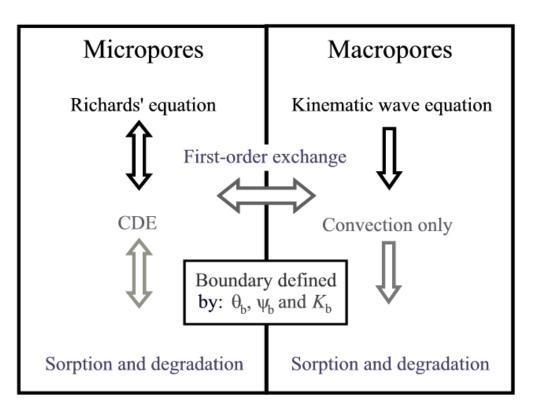


Frozen

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

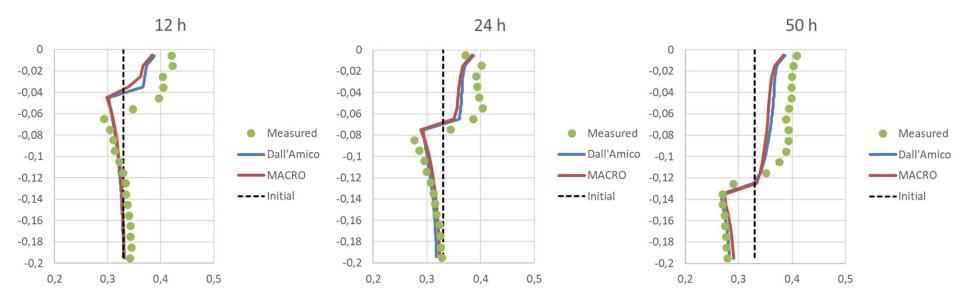
Hansson, K., J. Šimůnek, M. Mizoguchi, L.-C. Lundin and M. T. van Genuchten (2004). "Water Flow and Heat Transport in Frozen Soil." <u>Vadose Zone J. **3(2): 693-704.**</u>

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



Redistribution of water – freezing from the soil surface <u>Only soil matrix</u>

Initial conditions: Water content = 0.33; Soil temperature = $6.7 \degree C$ Top boundary condition: Temperature = $-6 \degree C$; No water flow Bottom boundary: No flow

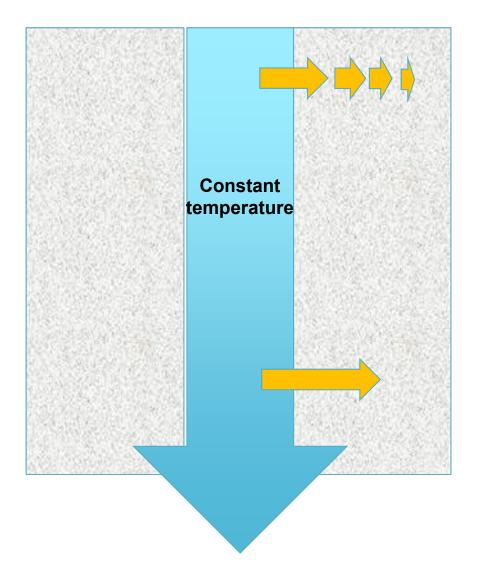


Mizoguchi, M. 1990, Water, heat and salt transport in freezing soils. PhD thesis (In Japanese), University of Tokyo.

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



Energy exchange between pore domains



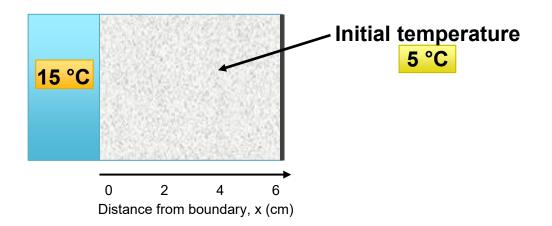
Heat conduction equation

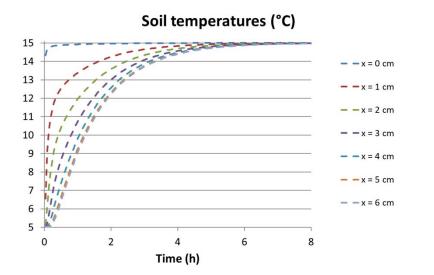
$$\frac{\partial C_{v}T}{\partial t} = \frac{\partial}{\partial x} \left(k_h \frac{\partial T}{\partial x} \right)$$

First-order approximation to the heat conduction equation

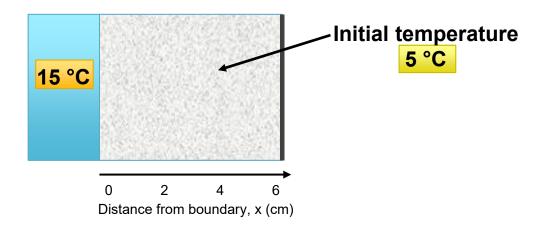
$$\frac{\partial C_{v}T}{\partial t} = \frac{G_{f}k_{h}S_{mac,tot}}{d^{2}}\left(T_{mic}-T_{mac}\right)$$

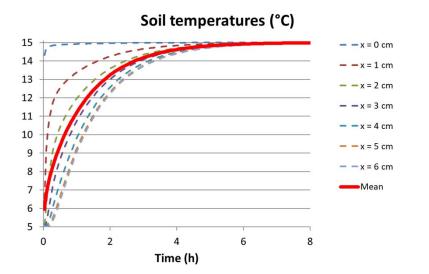




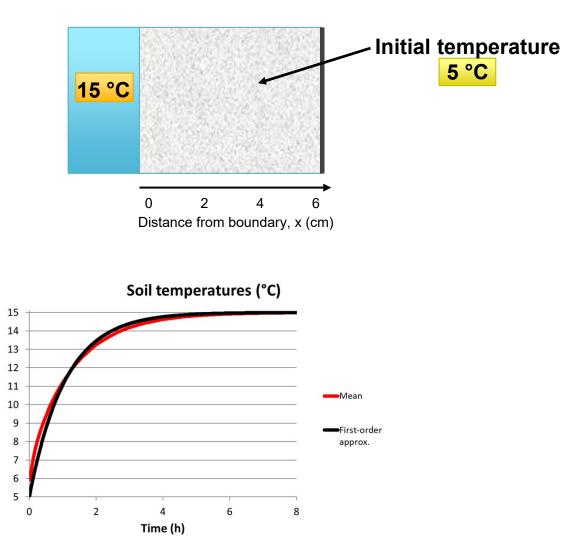




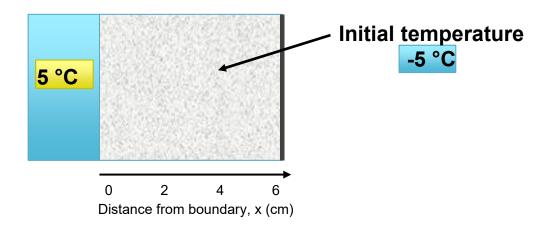


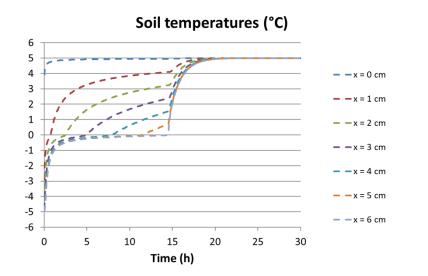




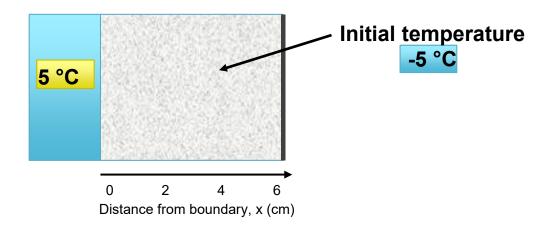


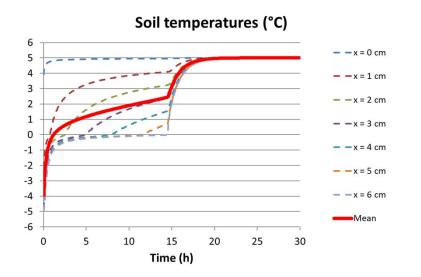




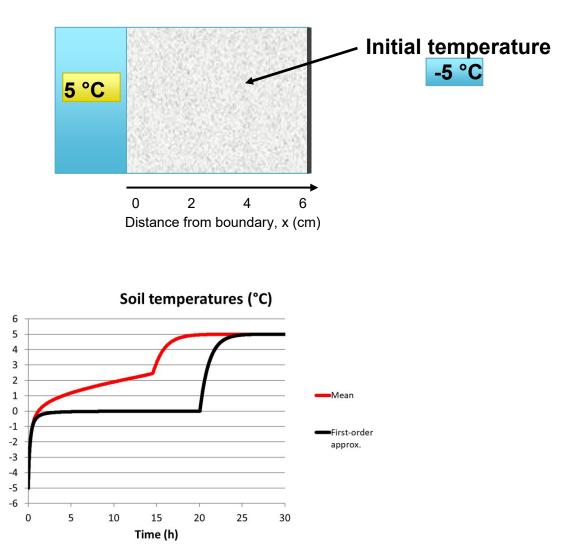






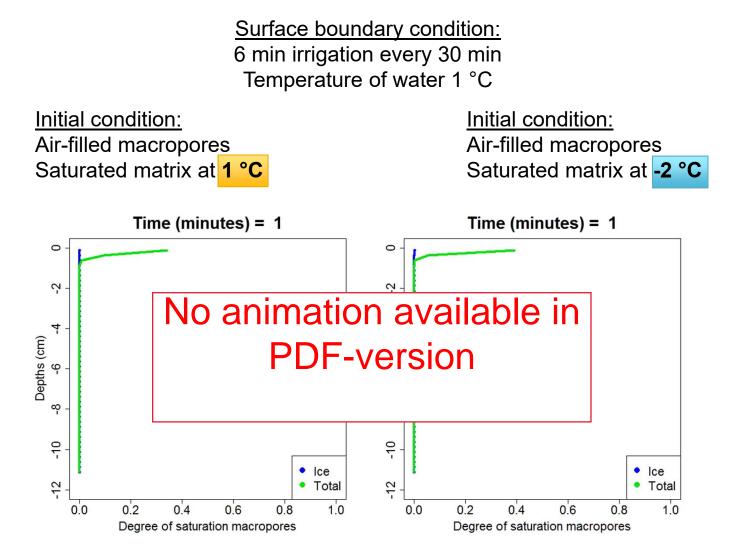








Water flow in macropores



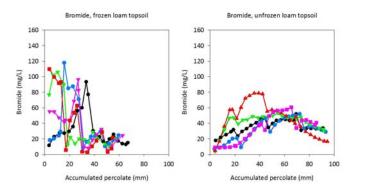


Conclusions...

- 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





Acknowledgements





Thanks for listening!