

Revisiting MACRO 5.2 Parameterization for EU & UK Drainage Scenarios

Gerald Reinken¹, Denis Weber², Michael Brauer²
¹Bayer AG Crop Science, Monheim, Germany ²Exponent Int. Ltd., Basel, Switzerland

Introduction

The MACRO model is a cornerstone of pesticide fate assessment within the FOCUS Surface Water (SW) framework, providing a physically based simulation of macropore flow and solute transport in structured soils. The MACRO model is also employed in the UK higher-tier drainflow assessment (HTDF). The original drainflow scenarios were parameterized using MACRO 4.3b, calibrated and validated against field data to ensure realistic hydrological behaviour (FOCUS, 1997).

With the release of MACRO 5.2 (FOCUS VC, 2012), several technical updates were implemented, including changes in numerical routines, parameter management, and batch-execution functionality. While these updates improve model flexibility and performance, early comparisons indicated that outputs for standard FOCUS SW scenarios may deviate from those generated with the earlier version, potentially affecting regulatory consistency.

Materials and Methods

A systematic approach has been initiated to evaluate and better harmonize MACRO 5.2 with well established FOCUS drainflow benchmarks. Presented are outcomes of ongoing work.

Step I: Problem definition: Exemplary MACRO test simulations for a pre-emergence herbicidal use in winter cereals (application rate = 200 g a.i./ha, DT₅₀ in soil = 48 d, DT₅₀ in water = 40 d, DT₅₀ in sediment = 1000 d, K_{OC} = 390 L/kg, 1/n = 0.87, TSCF = 0, Q₁₀ = 2.58, Walker exponent B = 0.7 or 0.49)

Step II: Detailed comparison of process implementation and parameterization between MACRO versions 4.3b and 5.2 based on respective manuals as well as model input and output files.

Step III: Comparison of considered soil hydrologic conductivity and water retention and resulting parameterization in MACRO.

Results

Step I: The results of exemplary FOCUS Step 3 and UK HTDF test simulations with the test substance demonstrate:

- MACRO 5.2 can result in significantly higher PEC_{sw} values (increase by a factor of 2 to 5) in FOCUS and UK scenarios.
- Modifying the Walker exponent B from 0.7 to 0.49 as a workaround cannot compensate for this increase.

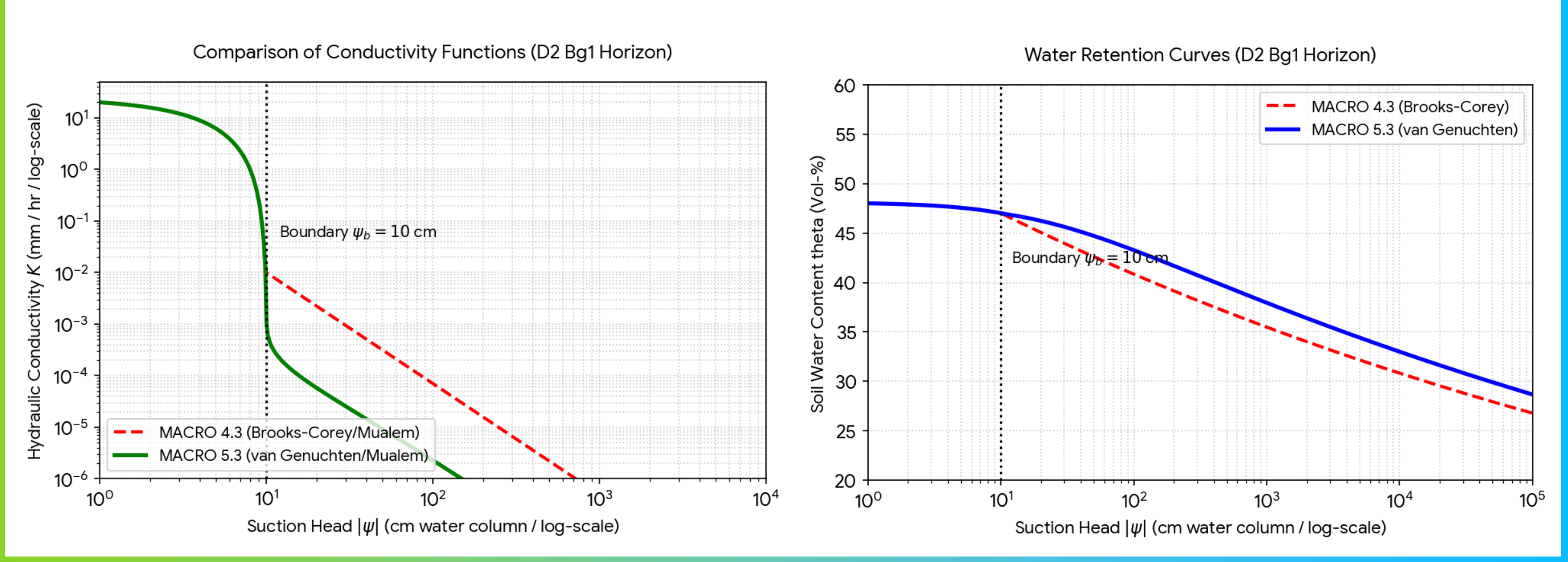
Step II: A detailed evaluation of the technical descriptions of the two model versions identified **major technical deviations**.

- Overview of changes introduced with MACRO 5.2:
- a) Adjusted numerical solver technique** (change from explicit with fixed time-stepping to implicit finite-difference procedure for the micropore = matrix domain)
 - b) Internal EVAPORATE calculation** (by Penman–Monteith instead of reading PET time series from file, used for UK HTDF but not used for FOCUS D)
 - c) Finer vertical resolution** (numerical layers increased from 15 to 60)
 - d) Use of modified van Genuchten equation** (instead of Mualem-type function for matrix hydraulic conductivity paired with Brooks-Corey retention in MACRO 4.3)

Results of comparative test simulations with MACRO 4.3b and MACRO 5.2					
Scenario	Waterbody	Macro 4	Macro 5	Macro 5	Ratio Macro 5 / Macro 4
FOCUS Step 3		Max PEC _{sw} (µg/L)			
		B=0.7	B=0.7	B=0.49	
D1	Ditch	4.74	7.98	7.87	1.66
D1	Stream	2.96	4.99	4.92	1.66
D2	Ditch	3.71	13.00	12.90	3.48
D2	Stream	2.34	8.12	8.08	3.45
UK HTDF					
Denchworth	medium	3.27	6.40	6.34	1.94
Denchworth	wet	1.82	9.42	9.29	5.11
Hanslope	medium	2.44	3.15	3.13	1.28
Hanslope	wet	0.93	4.22	4.17	4.48

- e) Newly introduced parameters** (due to changes in process implementation, such as van Genuchten, crop management, ...)
- f) Scenario-specific FRACMAC values** (fraction of sorption sites located in the macropore domain)
Changes since MACRO version 5.0:
- g) Modified Walker equation** with new lower limit (deviation from FOCUS: no degradation if soil moisture is < 0.5 θ_w [wilting point])
- h) Modified bottom boundary condition** (preventing any upward flow from groundwater into unsaturated soil profile)

Step III: Significant differences in the hydrologic properties of individual soil layers are evident (example below: D2 Bg1 horizon). This promotes **accelerated preferential flow**:
As the soil matrix saturates, it can no longer accommodate high-intensity inflows, so later pulses bypass the matrix and preferential macropore flow through structural cracks is activated earlier and more strongly. This is directly reflected in the table, where wet scenarios show the highest ratios (up to a factor of ~5).



Conclusions / Discussion

- Major changes in parameterization and process implementation exist between MACRO 4.3b and MACRO 5.2.
- Significant differences in the hydrologic characterization of individual soil layers may be a major reason of enhanced macropore flow and elevated PEC_{sw}.
- Next Steps: Use systematic MACRO 5.2 simulations to re-parameterize the model and improve agreement with 4.3b reference loads.

Take home message
MACRO 5.2 systematically increases drainflow PEC_{sw} by a factor of 2 to 5 compared to MACRO 4.3b. A re-parameterization is needed to ensure regulatory consistency.

Literature
- The MACRO Model (Version 4.3) Technical Description, Nicholas Jarvis - 2001
- MACRO 5.0: A model of water flow and solute transport in macroporous soil. Technical description, Mats Larsbo, Nicholas Jarvis - 2003
- Changes from earlier versions of MACRO 5. Mats Larsbo - 2011 (covers changes up to MACRO 5.2)

Note: The technical evaluation of the manuals was carried out based on a systematic review of the technical manuals and model I/O files, supported by AI-assisted literature/manual analysis.