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MACRO - Parameterisation for the FOCUS Groundwater Scenarios

About this document

The report on which this document is based is that of the FOCUS Groundwater Scenarios workgroup, which is an official guidance document in the context of 91/414/EEC [full citation is FOCUS (2000) "FOCUS groundwater scenarios in the EU review of active substances" Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference SANCO/321/2000 rev.2, 202pp]. This document does not replace the official FOCUS report. However, a need was identified to maintain the parameterisation of the models for the FOCUS groundwater scenarios in an up-to-date version controlled document, as changes become necessary. That is the purpose of this document.

Summary of changes made since the official FOCUS Groundwater Scenarios Report (SANCO/321/2000 rev.2).

New in Version 1.0

The only changes in this version compared with the original report are editorial ones.

New in Version 2.0

Updated to reflect changes in version 5.5.3.

New in Version 3.0

Updated to reflect changes in version 5.5.4.

1 Summary

MACRO 5 is a one-dimensional, non-steady state model of water flow and solute transport in a layered soil at the pedon/ field scale. The model describes a high-conductivity/low porosity macropore domain coupled to a low-conductivity/high porosity domain representing the soil matrix. Mass exchange between the domains is calculated with approximate, yet physically based, first order expressions. The model structure therefore enables quantitative evaluation of the impact of water flow and solute transport through macropores in structured soil. However, types of preferential flow other than through macropores are not simulated.

With respect to the FOCUS groundwater scenarios, MACRO was parameterised for the Châteaudun scenario only. MACRO includes the following processes:

-	Unsaturated water flow	Richards' equation in micropores, gravity flow in macropores
-	Root water uptake	Empirical sink term, water preferentially extracted from macropores
-	Seepage to drains	Seepage potential theory. Sink term in the vertical water flow equation. Drains are not simulated for the FOCUS groundwater scenarios.
-	Solute transport	Convection/dispersion equation in the micropores, mass flow only in the macropores
-	Mass exchange	Approximate first order rate equation for mass exchange of both solute and water
-	Sorption	Instantaneous equilibrium, Freundlich isotherm, sorption partitioned between micro- and macropores
-	Degradation	First-order kinetics, separate rate coefficients for four pools (solid and liquid, micro- and macropores).
-	Metabolism	One metabolite can be simulated at a time
-	Canopy interception and washoff	These routines are turned off, following FOCUS procedures.
-	Plant uptake	Plant uptake is calculated as a function of plant transpiration

MACRO does not (or not fully) include the following processes

-	Volatilisation	A lumped dissipation rate including volatilisation, photolysis etc. may be given for the leaves, but this option is not active in the FOCUS scenarios. Volatilisation from the soil is not included.
-	Surface runoff	Surface runoff of water and solute is only included in the sense that if the surface layer is saturated, the excess water and solute is lost to the profile. But it cannot be used to model runoff processes as such.

The main issue encountered during parameterisation was the parameterisation of macropore flow. The relevant parameters were given values based partly on the pedotransfer functions available in MACRO_DB, and partly on a rough calibration of the model on measured water flow data from lysimeters at Châteaudun (Villamblain). In the Châteaudun profile, macropore flow is assumed to be weak in the upper 25cm, strong between 25 and 60cm depth, and non-existent below 60cm.

In addition to the crop parameters specifically given for the FOCUS scenarios, a number of crop parameters had to be estimated. This concerns, among others, LAI at harvest, a root adaptability factor, maximum water interception by the crop, factors describing the change in

leaf area development over time, critical soil air content for root water uptake, a factor describing the distribution of the roots in the root zone, critical tension for root water uptake, and a correction factor for evaporation from wet canopy. The parameter set for the crops grown at Châteaudun is listed in Tables 3 and 4.

The reduction of substance reaching the soil surface due to crop interception is parameterised as follows. The user should input the dose actually reaching the ground, excluding the amount intercepted by the crop. The fraction intercepted is determined from the interception tables as described in the guidelines in Chapter 2.3 of the FOCUS report. Washoff is set to zero ensuring that only the amount of substance directly entering the soil contributes to leaching.

2 Introduction

A common shell program has been written for the MACRO model to run the single FOCUS groundwater scenario as well as the six FOCUS surface water scenarios developed for MACRO. The shell program is PC-based and written in Visual Basic. All parameter values defining the scenarios are contained in a number of Microsoft Access databases. For the single groundwater scenario at Châteaudun, the user simply selects a crop from the available list, and then sets options for the length of simulation (20, 40 or 60 years). Substance properties can also be defined interactively and stored in a separate database for later use. In-built calculation routines present the results of the simulations to the user in the correct format for FOCUS. It is possible to export simulation results to text files for further processing.

The scenario and parameter definitions are based on:

- **FOCUS DEFINITION** = General definitions made by the FOCUS working group
- **FOCUS SCENARIO SPECIFIC** = Definitions made by the FOCUS working group for a specific scenario
- **DEVELOPMENT DEFINITION** = Definitions made by the FOCUS working group specifically for the MACRO model.
- **USER INPUT** = Input defined by the user, through choices and selections made in the MACRO shell.

In case users wish to make subsequent higher tier assessments based on the defined scenarios, by modifying them, it is possible to save them to a MACRO 5.2 database and open the simulation from the MACRO 5.2 shell program.

3 Input files

The meteorological files are stored as binary formatted (*.bin* extension) files. They contain the following information:

Parameter and description		Value, source & comments
Rainfall file	czm6p.bin	
	Date	**FOCUS SCENARIO SPECIFIC**
	Precipitation (mm day^{-1})	**FOCUS SCENARIO SPECIFIC**
Evaporation file	czm6et.bin	
	Date	**FOCUS SCENARIO SPECIFIC**
	Potential evaporation (mm day^{-1})	**FOCUS SCENARIO SPECIFIC**
	Max daily temperature, (°C)	**FOCUS SCENARIO SPECIFIC**
	Min. daily temperature, (°C)	**FOCUS SCENARIO SPECIFIC**

4 Switches

Values of switches (= options) determine the type of simulation to be performed and the parameters required.

Technical Switches

Parameter and description		Value, source & comments
Averagex	Determines whether the output value is calculated as the value at the end of the interval (1) or the average value of a variable for a calculation interval (2).	2 is chosen. **DEVELOPMENT DEFINITION.**
Chapar	Allows the use of more than one parameter set during a simulation.	For most of the crops, one parameter set is chosen (OFF). However, for the crop with two growing seasons during the year, the switch is ON. **DEVELOPMENT DEFINITION** for each crop choice based on the FOCUS scenarios.
Driving	Specifies whether metabolites are being simulated	For all simulations without metabolites it is set to 0. For simulation of a metabolite, it is set to 1. **USER INPUT.**
Lisallv	General selection of output variables to summary file	All possible output variables are written to the summary file (2). **DEVELOPMENT DEFINITION**
Metabolite	Specifies whether a driving file for metabolites is to be produced.	This parameter is set to OFF if no metabolites of a certain substance are to be simulated. If metabolites are to be simulated, it is set to ON. When simulating the metabolite (Driving=1), it is set to OFF. **USER INPUT**
Validpg	Specifies whether there is comparison with measured data	As there is no comparison with measured data, this parameter is set to 0. **DEVELOPMENT DEFINITION**.

Model Specific Switches

Parameter and description		Value, source & comments
Boundary	Specifies the lower boundary condition for the column.	The groundwater depth is **FOCUS SCENARIO SPECIFIC**, the exact choice of lower boundary condition is a **DEVELOPMENT DEFINITION**. MACRO allows five different lower boundary conditions, namely 1) unit hydraulic gradient, 2) flux as an empirical function of water table height; 3) water table in the soil profile, 4) constant potential, and 5) lysimeter with free drainage. Due to the fact that the groundwater is at 12 m depth at Châteaudun, the constant potential gradient is selected as lower boundary condition.
Crop	Indicates the type of cover. The model allows bare soil conditions (1), annual crops (2), or perennial crops (3).	**FOCUS SCENARIO SPECIFIC**. The parameter is set to 2 or 3 depending on the crop.
Evaporate	Indicates the type of input given for calculation of potential evaporation.	As daily potential evaporation is given as input to the model, the value is set to 1. **DEVELOPMENT DEFINITION**.
Initial	Indicates which type of initial condition for water content is selected.	The initial condition is set as an equilibrium profile (1). Due to the six years of warming up period used in the simulations, the values are not critical for the simulation.
Irrigate	Indicates whether or not irrigation should be treated as rainfall.	As the substance is given as an irrigation, irrigation should be treated separately from rainfall (1). **DEVELOPMENT DEFINITION**.
Massunits	Allows selection of different mass units.	The units mg are selected as mg m^{-3} equals $\mu g\ l^{-1}$, which is an appropriate unit for the substance simulations. **DEVELOPMENT DEFINITION**
Rainfall	Specifies the type of rainfall record.	As daily rainfall is used, this parameter is set to 1. **DEVELOPMENT DEFINITION**.
Solute	Specifies the solute being simulated.	MACRO allows simulation of water and heat, pesticide, non-reactive solute or tritium. The parameter should be set to 2. **DEVELOPMENT DEFINITION.**
Tiledrain	Indicates presence or absence of tile drains.	As no tile drains are present in the Châteaudun scenario, this parameter is set to 2. (**FOCUS SCENARIO SPECIFIC** parameter).

5 Parameters

Soil profile

Parameter and description		Value, source & comments
Nlayer	Number of layers to be simulated	Set to 200 - **DEVELOPMENT DEFINITION**
Z(1-200)	Thickness in mm of the 200 layers	The division of the soil profile into numerical layers follow the same routines as in MACRO 5. (**DEVELOPMENT DEFINITION**)

Site

Parameter and description		Value, source & comments
ANNAMP	The temperature amplitude between the average temperature in January and July. (°C)	Calculated from the weather record to be 7.7 ^{o}C. **FOCUS SCENARIO SPECIFIC**.
ANNTAV	The average annual temperature (°C)	Calculated from the weather record to be 11. 9 ^{o}C. **FOCUS SCENARIO SPECIFIC**.
PHI	Site latitude	48.1 **(FOCUS SCENARIO SPECIFIC)**
RAINCO	Correction coefficient for rain.	For the scenarios it is assumed to be 1. **DEVELOPMENT DEFINITION**
RINTEN	A typical rainfall intensity for the area in question (mm hr^{-1}).	For southern England, a value of 2 mm/hr is realistic. The same value was selected for ChâteaudunChâteaudun. **DEVELOPMENT DEFINITION**
SNOWCO	Correction factor for snowfall.	For the scenarios it is assumed to be 1. **DEVELOPMENT DEFINITION.**
SNOWMF	This factor governs the rate of snowmelt.	Set to default, 4.5 mm degree^{-1} day^{-1}. Snow is not regarded to be important in ChâteaudunChâteaudun. **DEVELOPMENT DEFINITION**.

Initial/Boundary conditions

Parameter and description		Value, source & comments
BOTEN	Tension at the lower boundary of the profile (cm)	For groundwater at 12 m depth as defined for ChâteaudunChâteaudun, the value is calculated as (12 – 1.9 m = 10.1 m), assuming equilibrium conditions. The resulting tension at the bottom of the soil column is 1010 cm**. DEVELOPMENT DEFINITION** based on **FOCUS SCENARIO SPECIFIC** parameters.
CONCIN	Solute concentration at the bottom boundary	Set to zero (**FOCUS DEFINITION**)
SOILINIT	Initial concentration in the soil	Set to zero (**FOCUS DEFINITION**)
TEMPINI	Initial temperature in the soil profile.	Set to 10 °C. Due to the warming up period, the initial values are without importance for the simulation. **DEVELOPMENT DEFINITION**.

Solute transport

Parameter and description		Value, source & comments
AEXC	Excluded volumetric water content due to anion exclusion. (%)	Set to zero. **DEVELOPMENT DEFINITION**.
CONC	The solute concentration in rainfall	Set to zero. **FOCUS DEFINITION**
DIFF	The diffusion coefficient for the substance ($m^2 s^{-1}$)	**USER INPUT**. The default value is 5.0 E-10.
DV	Dispersivity (cm)	Set to 5 cm – **FOCUS DEFINITION**
FSTAR	The solute concentration factor for crop uptake of substance	**USER INPUT**. The default value is 0.5
ZMIX	Mixing depth for rainfall and soil moisture (mm).	Set to 1 mm (default). **DEVELOPMENT DEFINITION**.

Substance

Parameter and description		Value, source & comments
CANDEG	Dissipation rate coefficient on leaves (1/days)	0.2 (default value). This is irrelevant since the crop interception is set to zero (**FOCUS DEFINITION)**
DEGMAL	Degradation rate coefficient (1/days), at a moisture content of XMPOR and the temperature TREF, for the liquid phase in the macropores	**USER** INPUT for each horizon. Although MACRO internally uses XMPOR as the reference moisture for degradation, it has been ensured through the shell that the degradation value at pF2 is exactly equal to that used in the other FOCUS models.
DEGMAS	As above, for the solid phase in the macropores	**USER INPUT**, for each horizon.
DEGMIL	As above, for the liquid phase in the micropores.	**USER INPUT**, for each horizon.
DEGMIS	As above, for the solid phase of the micropores.	**USER INPUT**, for each horizon.
EXPB	Exponent of moisture corrected degradation (moisture relationship according to WALKER)	**USER INPUT** (0.49 = default value)
FCONVERT	Fraction of degraded parent compound converted to metabolite.	**USER INPUT**.
FEXT	Wash-off coefficient for the leaves (1/mm)	Set to zero. Irrelevant. **FOCUS DEFINITION**.
FRACMAC	The fraction of sorption sites in the macropores	0.02 (default value in model) **DEVELOPMENT DEFINITION**.
FREUND	Exponent of the Freundlich isotherm	**USER INPUT**
TREF	Reference temperature for substance degradation (^{o}C)	**USER INPUT**
TRESP	Exponent in the temperature response function (1/Kelvin)	**USER INPUT** (default value = 0.0948)
ZKD	Sorption distribution coefficient, $cm^3\ g^{-1}$	**USER INPUT**

Physical/Hydraulic properties

For the hydraulic parameters, the parameterisation of MACRO is different from the other models. The hydraulic parameters (retention curve and unsaturated hydraulic conductivity) were fitted both with the van Genuchten/Mualem and Brooks-Corey/Mualem models. The two fits produce very similar results for the micro-pore range of tensions, but rather different results near saturation. All required data are listed in Tables 1 and 2.

Parameter and description		Value, source & comments
ASCALE	Effective diffusion pathlength (mm)	Determined via the pedotransfer functions in MACRO DB, based on the description of soil structure. The values chosen are 10 (0-25 cm), 75 (25-60 cm), 1 (60-120 cm) and 4 (120-190 cm). **DEVELOPMENT DEFINITION**
CTEN	Tension defining the macropore-micropore boundary (cm)	**DEVELOPMENT DEFINITION** The value may be identified from measured unsaturated hydraulic conductivity curves, as the point where the curve „breaks". The Villamblain data did not cover the tension range close to saturation. The values were chosen to give 1) a good fit to the unsaturated conductivity, with 2) a value as close to saturation as possible (if CTEN moves too far away from saturation, the model assumption of gravity flow in macropores breaks down. The value is given as h_b in the Table 2.
GAMMA	Bulk density (g/cm^3)	**FOCUS SCENARIO SPECIFIC**
KSATMIN	The saturated hydraulic conductivity ($mm\ hr^{-1}$)	Given in Table 1 as Ksat for Châteaudun. **FOCUS SCENARIO SPECIFIC**.
KSM	The saturated hydraulic conductivity of the micropores ($mm\ hr^{-1}$)	K_b in Table 2. **DEVELOPMENT DEFINITION**
RESID	Residual moisture content (%)	Given in Table 1 as θ_r for Châteaudun. **FOCUS SCENARIO SPECIFIC**.
TPORV	Saturated water content (%)	Given in Table 1 as θ_s for Châteaudun. **FOCUS SCENARIO SPECIFIC**.
WILT	Wilting point (%)	**FOCUS SCENARIO SPECIFIC**, Given in Table 2 as water content at 1600kPa for Châteaudun.
XMPOR	Saturated water content of micropores (%)	θ_b in Table 1. **DEVELOPMENT DEFINITION**.
ZA	Parameter relevant for simulation of shrinkage	Set to 1. Irrelevant for the simulation
ALPHA	van Genuchten's α	α in Table 1. **DEVELOPMENT DEFINITION**
N	Van Genuchten's N	*N* in Table 1. **DEVELOPMENT DEFINITION**
ZM	Tortuosity factor, micropores	λ in Table 1. **DEVELOPMENT DEFINITION**.
ZN	Tortuosity factor, macropores	The value of ZN was chosen based on a very approximate calibration against measured water discharges from the Villamblain lysimeters. A value of 3.0 is selected down to 60 cm, 2 in the deeper layers. **DEVELOPMENT DEFINITION**
ZP	Indicates presence or absence of shrinkage	Set to 0 = no shrinkage. **DEVELOPMENT DEFINITION**.

Crop

Crop parameters at Châteaudun are listed in Tables 2 and 3.

Parameter and description		Value, source & comments
BETA	Root adaptability factor	**DEVELOPMENT DEFINITION** for each crop.
CANCAP	Maximum water interception by the crop (mm)	CANCAP may be calculated as approximately 0.5 * LAI max. However, in some cases, values were selected to match the FOCUS surface water scenarios. **DEVELOPMENT DEFINITION**.
CFORM	Leaf development form factor for the period from emergence to maturity	The values given in Table 2 are derived from visual comparisons between published growth curves and fitted curves. **DEVELOPMENT DEFINITION**.
CRITAIR	Critical soil air content for root water uptake (%)	Kept at default (= 5). This value is not too far from the difference between field capacity and saturation weighted through the first meter of the profile, and also the default value used for the FOCUS surface water group. **DEVELOPMENT DEFINITION**.
DFORM	Leaf senescence form factor for the period from maturity to harvest	The values given in Table 2 are derived from visual comparisons between published growth curves and fitted curves. **DEVELOPMENT DEFINITION**.
IDMAX	The day of maturity of the crop	**FOCUS SCENARIO SPECIFIC**
IDSTART	The day of emergence of the crop	**FOCUS SCENARIO SPECIFIC**
IDHARV	The day of harvest of the crop	**FOCUS SCENARIO SPECIFIC**
LAIHARV	LAI at harvest	The values given in Table 2 are derived from published data. **DEVELOPMENT DEFINITION**
LAIMAX	LAI at maturity	**FOCUS SCENARIO SPECIFIC**
LAIMIN	The LAI at the date ZDATEMIN	For spring-sown crops the value is close to zero, for winter crops it is the LAI value during early spring. **DEVELOPMENT DEFINITION**.
ROOTINIT	The root depth at the date ZDATEMIN (m).	Set to the values given in Table 2. For summer crops the value is close to zero, for winter crops it is the root depth during early spring. **DEVELOPMENT DEFINITION**.
ROOTMAX	Maximum root depth, m.	**FOCUS SCENARIO SPECIFIC**.
RPIN	Percentage of the root length in the top 25 % of the root depth.	Set to 60 % (model default). **DEVELOPMENT DEFINITION**.
WATEN	Critical tension for root water uptake (m)	Given in Tables 2 and 3 for the different crops. **DEVELOPMENT DEFINITION**.
ZALP	Correction factor for evaporation from wet canopy.	Given in Tables 2 and 3 for the different crops. **DEVELOPMENT DEFINITION**
ZDATEMIN	The day number corresponding to LAIMIN and ROOTINIT	Values given in Table 2, set one day after emergence for summer crops and as day 90 for the winter crops. The growth is expected to increase significantly after this date. **DEVELOPMENT DEFINITION**.
RI50	The solar radiation that reduces stomatal conductance by 50% (W/m2)	Default values from MACRO 5. **DEVELOPMENT DEFINITION**
VPD50	The vapour pressure deficit that reduces stomatal conductance by 50% (Pa)	Default values from MACRO 5. **DEVELOPMENT DEFINITION**

Irrigation

This is used as a way to apply the substance to the soil

Parameter and description		Value, source & comments
AMIR	Amount of irrigation water applied (mm) in which the substance is mixed.	**DEVELOPMENT DEFINITION** 1000 l/ha = 1 m^3/10,000 m^2 = 0.1 mm is used
CONCI	Concentration of the substance in the irrigation water (mg m^{-3})	**USER INPUT** Calculated from the user-defined dose and AMIR
CRITDEF	Specification of criteria for irrigation	As there is no automatic irrigation, the value is set to (-1). **DEVELOPMENT DEFINITION**
IRRDAY	Day of irrigation (Day of substance application)	**USER INPUT**
IRREND	Time when the irrigation ends.	Given as hours and minutes as decimal fraction. Set to 9.2. **DEVELOPMENT DEFINITION**
IRRSTART	Time when the irrigation starts	Given as hours and minutes as decimal fraction. Set to 9. **DEVELOPMENT DEFINITION**
NIRR	Number of irrigations	**USER INPUT**
ZFINT	The fraction of the substance which is intercepted	**FOCUS DEFINITION**. ZFINT is set to zero. This solution is also recommended for the other models. Crop interception must be estimated manually, from the table in the FOCUS report, and subtracted from the specified dose.

6 Output specification

Output variables are selected to allow calculation of a water-and substance balance for a 1 m profile and for the full profile, as well as for calculating target quantities for EU registration purposes. Daily values of each variable are stored in the output *.bin* files.

Miscellaneous (water)

Parameter and description		Value, source & comments
WFLOWOUT	Water flow rate out of layer from macropores (mm hr^{-1})	Specified for layer at the output depth
WOUT	Water flow rate out of layer from micropores (mm hr^{-1})	Specified for layer at the output depth

Water balance

Parameter and description		Value, source & comments
CCET	Accumulated actual evapotranspiration (mm)	
PRECIRA	Accumulated precipitation and irrigation (mm)	
TRUNOFF	Accumulated surface runoff (mm)	
TSTOREMI	Total water storage in micropores through the whole profile (mm)	The figure relates to the full profile and not the water balance at 1 m depth.
TSTOREMA	Total water storage in macropores through the whole profile (mm)	The figure relates to the full profile and not the water balance at 1 m depth.
TFLOWOUT	Total accumulated percolation (mm) (micropores and macropores)	The figure relates to the bottom of the profile, and not to the water balance at 1m depth.

Miscellaneous, other

Parameter and description		Value, source & comments
DEGMAC	Solute degraded in soil macropores (mass m^{-2} h^{-1})	Only used as input for metabolite simulation
DEGMIC	Solute degraded in soil micropores (mass m^{-2} h^{-1})	Only used as input for metabolite simulation
SFLOW	Solute flow rate out of layer, micropores (mass m^{2} h^{-1})	For the result layer only
SFLOWOUT	Solute flow rate out of layer, macropores (mass m^{2} h^{-1})	For the result layer only

Solute balance

Parameter and description		Value, source & comments
TADMA	Solute storage in profile, macropores only, solid phase (mass m^{-2})	
TADMI	Solute storage in profile, micropores only, solid phase (mass m^{-2})	
TDEG	Accumulated total degradation in the soil (mass m^{-2})	For this parameter, the value for the upper meter and for the profile is identical, due to the fact that degradation is specified for the upper meter only.
TUPT	Accumulated uptake of solute by crop, (mass m^{-2})	If the root depth is less than one meter, the value for the profile is identical to the value for the upper meter.
TCAM	Solute storage in macropores in the liquid phase, for the profile (mass m^{-2})	
TPAM	Solute storage in micropores in the liquid phase for the profile (mass m^{-2})	
TSOUT	Accumulated solute leaching (total for macro- and micropores) (mass m^{-2})	
TSRUN	Accumulated amount of solute lost in runoff (mass m^{-2})	

7 Run specification

The run specification should be daily outputs, with user start time given as 1901/01/01 and user specified end time, depending on the length of the simulation (26, 46 or 66 years).

Table 1 Soil hydraulic properties, Van Genuchten/Mualem parameters (restricted form, m=1-1/n)

depth	θ_s	θ_b	θ_r	α	n	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	10kPa $m^3\ m^{-3}$	1600kPa $m^3\ m^{-3}$	$m\ s^{-1}$ $*10^{-6}$	-	mm
0-25	0.43	0.41	0.0	5.00	1.080	0.374	0.253	20.00	0.50	30.25
25-50	0.44	0.43	0.0	5.00	1.095	0.372	0.235	30.00	0.50	34.25
50-60	0.44	0.43	0.0	5.00	1.095	0.372	0.235	50.00	2.50	13.70
60-100	0.44	0.43	0.0	1.50	1.160	0.386	0.185	12.00	-2.00	80.40
100-120	0.44	0.43	0.0	1.50	1.160	0.386	0.185	12.00	-2.00	-
120-190	0.49	0.47	0.0	1.07	1.280	0.417	0.116	9.06	-1.50	-
190-260	0.42	0.40	0.0	1.91	1.152	0.362	0.176	14.81	-1.18	-

[@] Plant available water in the soil layer.
Plant available water in the top 1 m is 158.6 mm.

Table 2 Soil hydraulic properties, Brooks-Corey/Mualem parameters

depth	θ_b	θ_r	h_b	b	Water content		K_b	λ	AW[@]
cm	$M^3\ m^{-3}$	$m^3\ m^{-3}$	m	-	10kPa $m^3\ m^{-3}$	1600kPa $m^3\ m^{-3}$	$mm\ h^{-1}$	-	mm
0-25	0.41	0.0	0.2	0.07	0.366	0.258	0.25	-0.50	27.00
25-50	0.43	0.0	0.2	0.09	0.372	0.237	0.50	-0.50	33.75
50-60	0.43	0.0	0.2	0.09	0.372	0.237	1.00	1.50	13.50
60-100	0.43	0.0	0.4	0.14	0.378	0.188	1.00	-4.00	76.00
100-120	0.43	0.0	0.4	0.14	0.378	0.188	1.00	-4.00	-
120-190	0.47	0.0	0.3	0.19	0.374	0.150	3.25	-3.50	-
190-260	0.40	0.0	0.3	0.14	0.338	0.176	1.00	-3.50	-

Note: K_{sat} and θ_s are the same as for the Mualem/van Genuchten fit shown in Table B.1.
[@] Plant available water in the soil layer.
Plant available water in the top 1 m is 150.3 mm.

Table 3 MACRO parameters for the annual crops for Châteaudun.

	Crop												
Parameter	apples	vines	**potatoes**	**sugar beet**	**cabbage**	**carrots**	**maize**	**onion**	**peas**	**spring cereals**	**tomatoes**	**winter cereals**	**oil seed rape (w)**
Crop	2	2	2	2	2	2	2	2	2	2	2	2	2
Chapar					on	on							
Date					197	180							
Beta	0.2	0.2	0.5	0.2	0.5	0.5	0.2	0.5	0.5	0.2	0.5	0.1	0.1
Cancap	4	3	2	2.5	2	2	3	2	2	2	2	3	3
Cform	1.5	1.5	1.7	1.7	1.5	1.5	1.7	1.5	1.7	2	1.3	2	2
Critair	5	5	5	5	5	5	5	5	5	5	5	5	5
Dform	0.7	0.7	0.3	1	1	1	0.3	1	0.3	0.3	0.3	0.2	0.2
IDMax	151	212	166	196	151/248	110/222	227	181	158	161	181	151	110
IDStart	91	91	120	106	110/212	69/191	121	115	95	69	130	299	250
Iharv	274	305	244	288	196/288	151/263	274	244	227	201	237	196	191
Laihar	0.01	0.01	2	5	3	3	2	3	3	2	3	2	2
Laimax	4	6	4	5	3	3	4.5	3	4	5	6	7.5	4
Laimin	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.3	1	1
Rootinit	1.89	1.89	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.1	0.2	0.2
Rootmax	1.9	1.9	0.6	1	0.6	0.8	0.8	0.6	0.6	0.6	0.8	0.8	1
Rpin	60	60	75	67	75	75	67	75	67	60	67	60	60
Waten	20	20	10	20	10	10	20	10	10	20	10	50	50
Zalp	3	2	1	1	1	1	1.5	1	1	1	1	1	1
Zdatemin	92	92	121	107	111/213	70/192	122	116	96	70	131	90	90
RI50	50	50	50	50	50	50	50	50	50	50	50	50	50
VPD50	50	50	50	50	50	50	50	50	50	50	50	50	50

Table 4 MACRO crop parameters for grass/alfalfa

Parameter	Value
Crop	3
Chapar	OFF
Beta	0.2
Cancap	2
Critair	5
Laic	5
Rootdep	0.5
Rpin	67
Waten	20
Zalp	1
Hcrop	0.2
RSURF	50

Table 5 Solute-related parameters : fixed for all substances in FOCUS

Parameter	Value
Aexc	0
Conc	0
Dv	5
Zmix	1
Candeg	0.2
Fext	0
Fracmac	0.02
Zfint	0

Table 6 User-defined properties : dummy substances A, B, C and its metabolite, and D

	Substance				
Parameter	**A**	**B**	**C**	**metabolite**	**D**
Diff	5.00E-10	5.00E-10	5.00E-10	5.00E-10	5.00E-10
Fstar	0.5	0.5	0.5	0.5	0.5
[a]Degmal(1-4)	0.0125	0.0375	0.0375	0.00750	0.0375
[a]Degmal(5-8)	0.00639	0.01918	0.01918	0.00385	0.01918
[a]Degmal(9-12)	0.00379	0.01137	0.01137	0.00228	0.01137
[a]Degmal(13-15)	0	0	0	0	0
Expb	0.7	0.7	0.7	0.7	0.7
Fconvert				0.53	
Freund	0.9	0.9	0.9	0.9	0.9
Tref	20	20	20	20	20
Tresp	0.079	0.079	0.079	0.079	0.079
K_{oc}[b]	103	17	172	52	60

[a] Degmas, Degmil, and Degmis receive the same values

[b] ZKD for individual horizons calculated as $f_{oc}*K_{oc}$

8 References

2003:6 Larsbo, M. & Jarvis, N. MACRO 5.0. A model of water flow and solute transport in macroporous soil. Technical description. 47 pages. ISBN: 91-576-6592-3