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PEARL - 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.

1 Summary

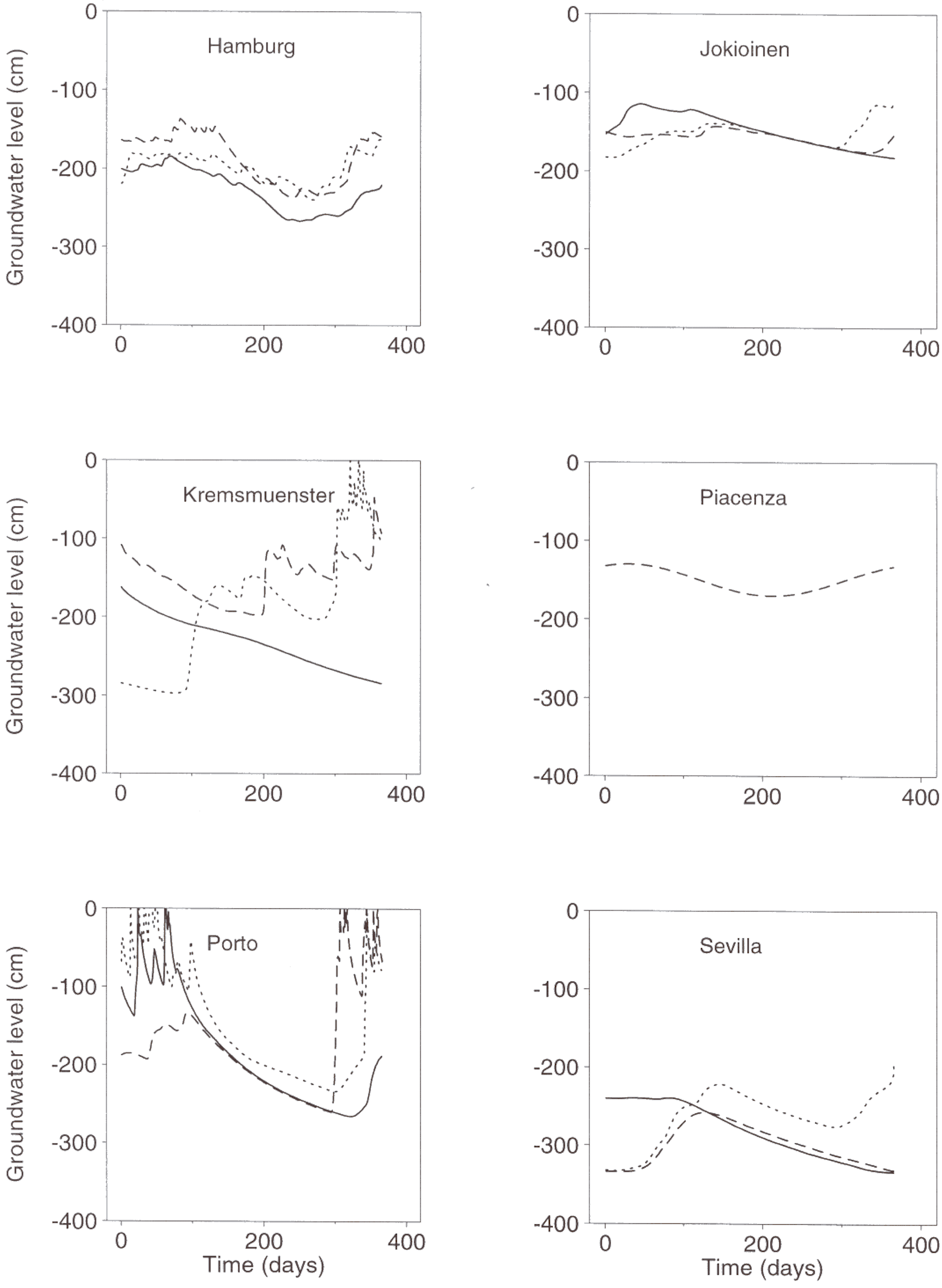
PEARL (Pesticide Emission Assessment at Regional and Local scales) is a consensus model developed by two Dutch institutes (RIVM and Alterra Green World Research) in close co-operation (Leistra at al, 2001). It is based on PESTLA (PESTicide Leaching and Accumulation; version 1: Boesten & Van der Linden, 1991; version 3.4:Van den Berg and Boesten, 1999) and PESTRAS (PEsticide TRansport Assessment. Tiktak et al., 1994; Freijer et al., 1996), the latter being a modification of PESTLA version 1. PEARL is based on (i) the convection/dispersion equation including diffusion in the gas phase with a temperature dependent Henry coefficient, (ii) a two-site Freundlich sorption model (one equilibrium site and one kinetic site), (iii) a transformation rate that depends on water content, temperature and depth in soil, (iv) a passive plant uptake rate. The model includes formation and behaviour of transformation products and describes also lateral pesticide discharge to drains (but drainage is switched off for the FOCUS scenarios). PEARL does not simulate preferential flow. Volatilisation from the soil surface is calculated assuming a laminar air layer at the soil surface. PEARL uses an explicit finite difference scheme that excludes numerical dispersion (the dispersion length was set to 5 cm).

For the FOCUS scenarios, the default option is to ignore long-term sorption kinetics (i.e. zero sorption coefficient for the kinetic sorption site in PEARL). However, if long-term sorption data are available for a compound, these can be used to estimate the kinetic sorption parameters in PEARL (sorption coefficient and desorption rate constant).

PEARL does not simulate water flow and soil temperatures itself but uses the Soil Water Atmosphere Plant (SWAP) model version 2.0 for that purpose. In SWAP, flow of water is described with Richard's equation using a finite implicit difference scheme (Van Dam et al., 1997). SWAP can handle a wide variety of hydrological boundary conditions. Soil evaporation and plant transpiration can be calculated via multiplying a reference evapotranspiration rate with soil and crop factors. SWAP can simulate groundwater levels that fluctuate in response to the rainfall input. The groundwater level can also be introduced as a time table (option used for the Piacenza scenario). Figure 1 shows examples of yearly fluctuations in groundwater levels as calculated with SWAP for all relevant locations (excluding Châteaudun, Okehampton and Thiva because their groundwater levels are deeper than 5 m). For the FOCUS scenarios, crop growth is simulated with SWAP using a simple growth model that assumes a fixed length of the growing season. In this growth model, both the leaf area index and the rooting depth are a function of the development stage of the crop.

SWAP describes flow of heat with Fourier's Law with a finite implicit difference scheme. The thermal properties are a function of porosity and water content and are therefore a function of time and soil depth.

Figure 1 Examples of yearly fluctuations in groundwater level for FOCUS scenarios simulated with SWAP for PEARL. Heavily dashed lines are for average years, solid lines for dry years and lightly dashed lines for wet years. All simulations are for potatoes assuming no irrigation.

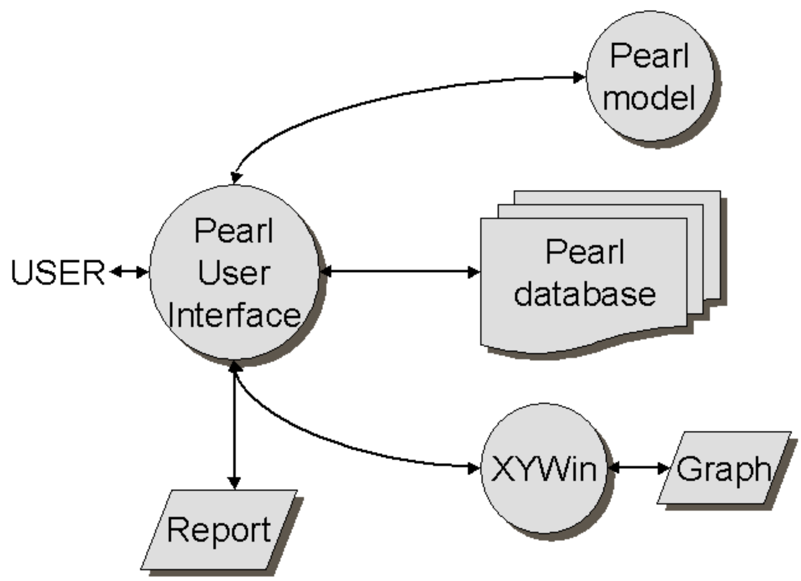


2 Parameterisation of PEARL

The Pesticide Emission Assessment for Regional and Local Scales model (PEARL) simulates the behaviour of substances in soil (Leistra et al., 2001; Tiktak et al., 2000). PEARL does not simulate water flow and soil temperatures, but uses output from the Soil Water Atmosphere (SWAP) model, so the software package for simulation consists of two models: SWAP and PEARL. Thus the simulation of leaching to groundwater with PEARL requires that first the hydrology of the soil system during the simulation period is computed with SWAP. Daily SWAP output is written a file which is one of the input files needed for PEARL. However, the user has only to specify input to PEARL: the PEARL model itself organises the input for the SWAP model.

The PEARL User Interface was developed as a user-friendly environment for running FOCUS scenarios. The interface is an integrated environment for data storage and data retrieval, model control and viewing of output data (Figure 2).

Figure 2. Overview of the PEARL modelling system



The user interface is linked to a relational database for easy data access. It generates the input files for the PEARL model and calls the model. Summary outputs are transferred back to the PEARL database where they can be accessed. More comprehensive model outputs can be viewed with a separate graphical program, *XYWin*. Figure 3 shows the main screen of the user interface (see Tiktak et al., 2000 for a detailed description of the PEARL User Interface).

The FOCUS input is stored in the database in such a way that all data are locked that should not be changed by the user. The user can generate a FOCUS scenario for a desired crop-location combination with a wizard as shown in Figure 4 (see Tiktak et al., 2000, for detailed instructions).

Figure 3 Main screen of PEARL User Interface

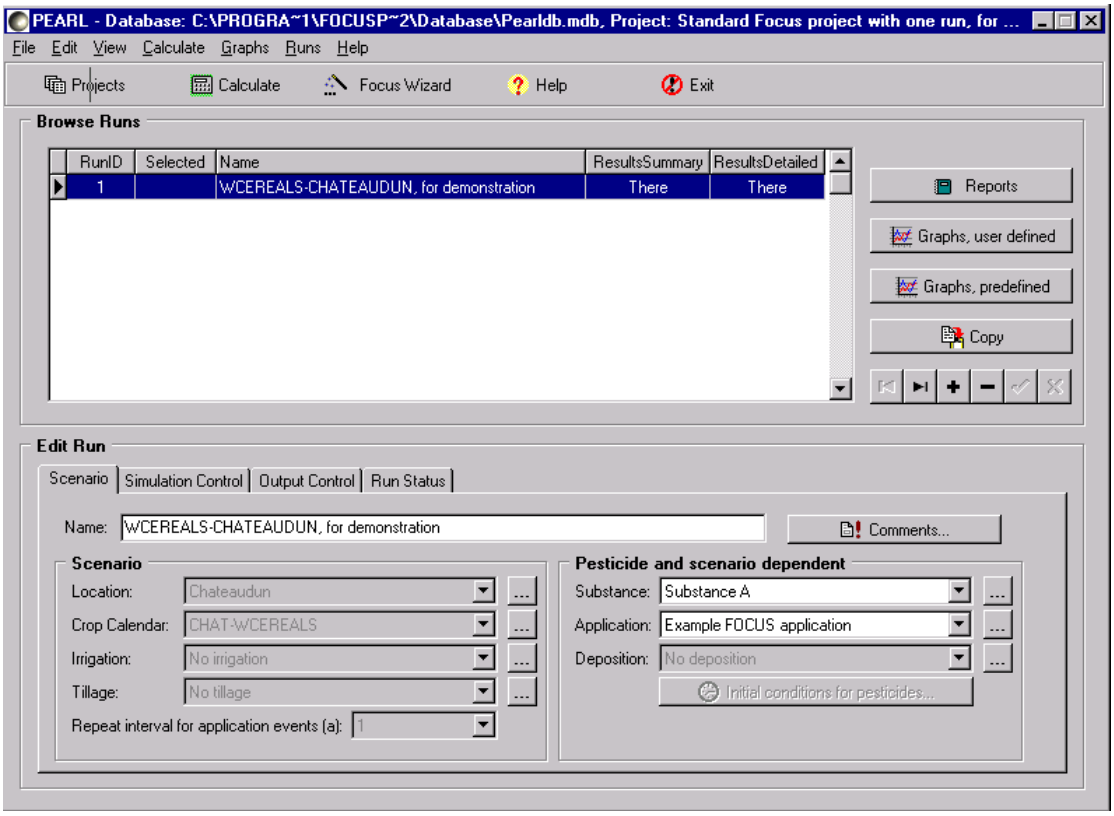
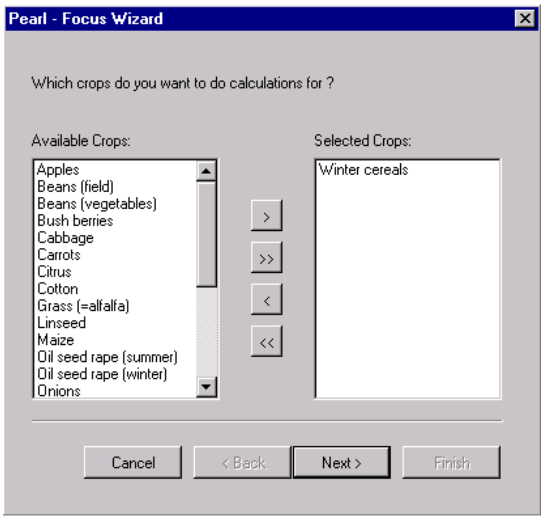
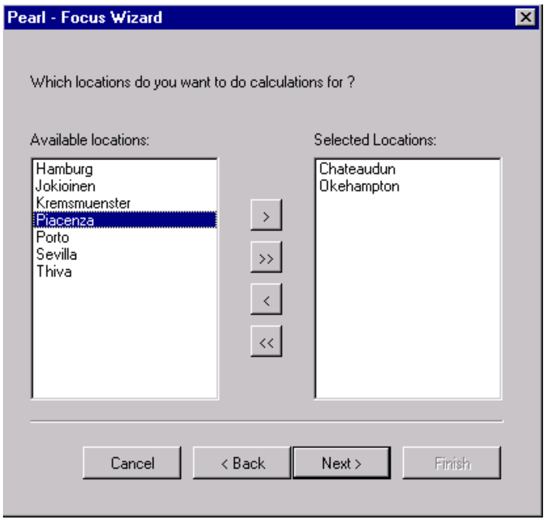


Figure 4 Part of the FOCUS wizard of PEARL User Interface





2.1 General description of PEARL input

Soil system

For each FOCUS location, the top 0.5 m layer of the soil system consists of compartments with a thickness of 0.025 m. If the boundary falls within a horizon, then the whole horizon consists of compartments of 0.025 m. Below this depth up to a soil depth of 1.0 m the soil profile consists of compartments of 0.05 m. Below 1.0 m the soil system consists of compartments with a thickness of 0.10 m.

The soil hydraulic functions are described with the analytical function of Mualem – Van Genuchten. The values of the parameters in this function have been specified by the FOCUS workgroup for each FOCUS location-soil layer combination. For all 9 FOCUS soil profiles, the composition of each layer, i.e. the clay, silt and sand fractions and the organic matter fraction, has also been specified by the FOCUS workgroup. Each soil layer is assumed to be homogeneous, so no preferential flow and flow through soil cracks occurs.

The potential evaporation from bare soil is calculated from the reference potential evapotranspiration by multiplication with a factor for bare soil. In the current version of SWAP, this factor is constant during the time the soil is bare. The FOCUS workgroup has set the value of this factor to 1.0.

The reduction of the potential evaporation from bare soil is described using the model by Boesten and Stroosnijder (1986). This model contains one parameter, beta. Boesten (1986, p. 63-64) reviewed beta values derived from literature and concluded that beta is usually in the range from 2 to 3 $mm^{1/2}$ and is no function of soil texture. Therefore we used a beta value of 2.5 $mm^{1/2}$ (corresponding with 0.79 $cm^{1/2}$).

The bottom boundary condition of the soil system depends on the average groundwater level. If the groundwater level is within the simulated soil profile then the course with time of the groundwater level is described. If the ground water level is below the simulated soil profile then a fixed groundwater level is assumed. At the start of each simulation, the pressure head in each compartment is assumed to be in hydrostatic equilibrium with the initial groundwater table.

Crop

In SWAP 2.0, the growth of the crop is expressed as a function of the development stage (DVS), which ranges from 0.0 (at crop emergence) to 2.0 (at the end of the crop cycle). At development stage 1.0 the crop reaches maturity. The crop growth can be simulated with a detailed or a simple crop model. For the FOCUS leaching scenarios, the simple crop model was used in all cases. Using this model, a fixed length of the growing cycle was selected. The length of the crop cycle is defined by the day of emergence and the day of the harvest as specified for each site-crop combination by the FOCUS work group. Thus, the same duration of the crop cycle was used for all simulated years within one scenario. In a fixed growth cycle the development stage increases linearly from 0.0 to 2.0 between the emergence of the crop and the end of the crop cycle (harvest).

The potential evapotranspiration is calculated from the reference potential evapotranspiration by multiplication with a crop factor for a dry canopy that completely covers the soil. In the current version of SWAP, the crop factor can be varied during the crop cycle. The crop factors used are those specified by the FOCUS workgroup. Daily values of the reference potential evapotranspiration are taken from the weather files as prepared by the FOCUS workgroup. The potential evapotranspiration is separated into the potential transpiration and potential evaporation on the basis of the leaf area index (LAI).

The irrigation data sets for 6 crop(group)s for the 4 locations where irrigation is possible (Châteaudun, Piacenza, Sevilla and Thiva) are those prepared by the FOCUS workgroup.

Weather

The daily weather data for all 9 locations have been extracted from the MARS dataset by the FOCUS workgroup.

2.2 Description – PEARL INPUT

As described before, the normal procedure is to generate FOCUS input via the database that is part of the PEARL User Interface. This interface produces at run time three ASCII input files:
1. X.PRL containing all soil and substance input parameters with X as the run identification
2. Y. MET containing meteorological input in which Y is the name of the meteorological station
3. Y.IRR containing irrigation input for the same location.

Below we specify the input in these three input files. The scenario and parameter definitions are based on:
1) **FOCUS DEFINITION** = Definitions made by the FOCUS working group
2) **FOCUS SCENARIO SPECIFIC** = Definitions made by the FOCUS group for a specific scenario
3) **DEVELOPMENT DEFINITION** = Definitions made during the PEARL FOCUS files development
4) **USER INPUT** = Input to be specified by the user in the PEARL FOCUS database.

X.PRL file

Parameter and description		Value, source & comments
Section 1: Control Section		
FocusGUIVersion	Version number of the GUI	Set to 1. **DEVELOPMENT DEFINITION**
FocusDataBaseVersion	Version number of the database	Set to 1. **DEVELOPMENT DEFINITION**
ScreenOutput	Output to screen	Set to Yes. **DEVELOPMENT DEFINITION**
TimStart TimEnd	Starting time of simulation End time of simulation	Specified (dd-mm-yy) for the 26, 46 or 66 year scenario. **FOCUS SCENARIO SPECIFIC**
AmaSysEnd	Stopcondition (kg.ha^{-1})	Set to 0. **DEVELOPMENT DEFINITION**
ThetaTol	Maximum difference in water content between iterations	Set at the default value of 0.001 (m^3.m^{-3}). **DEVELOPMENT DEFINITION**
DelTimPrn	Print interval (d)	Set to 100 d. **DEVELOPMENT DEFINITION**
RepeatHydrology	Repeat the same hydrology each year	Set to No. **DEVELOPMENT DEFINITION**
OptHyd	Hydrology simulation option	OptHyd set to Online, SWAP is called by PEARL and subsequently reads the SWAP output to compute the substance behaviour in soil. **DEVELOPMENT DEFINITION**

DelTimSwaMin Minimum time step DelTimSwaMax Maximum time step	The values for the minimum and maximum time steps for the discretization of the Richards' equation are taken to be 5.0 E-7 d and 0.1 d, respectively. **DEVELOPMENT DEFINITION**
OptDelOutput Option to delete detailed output	Set to No. **DEVELOPMENT DEFINITION**
PrintCumulatives Option to output cumulative data	Set to Yes. **DEVELOPMENT DEFINITION**
Section 2: Soil Section	
SoilTypeID Identification of soil type	The name consists of the first four letters of the name of the FOCUS location with the suffix '_S' **DEVELOPMENT DEFINITION**
Location	The name of the FOCUS location **DEVELOPMENT DEFINITION**
Table SoilProfile Table defining the soil profile	Specify for each horizon: 1) The horizon number [1|10] **FOCUS SCENARIO SPECIFIC**, 2) Depth of the lower boundary (m) **FOCUS SCENARIO SPECIFIC**, 3) The number of soil compartments [1|500] **DEVELOPMENT DEFINITION.** The nodes are distributed evenly over each horizon.
Table horizon SoilProperties Table specifying the soil composition for each horizon	Specify for each soil horizon: 1) the mass content of sand, expressed as a fraction of the mineral soil ($kg.kg^{-1}$) [0|1], 2) the mass content of silt, expressed as a fraction of the mineral soil ($kg.kg^{-1}$) [0|1], 3) the mass content of clay, expressed as a fraction of the mineral soil ($kg.kg^{-1}$) [0|1], 4) the organic matter mass content ($kg.kg^{-1}$) [0|1], and 5) the pH-KCl [1,13]. The format [x,y] is used to specify the acceptable range (i.e. from x to y) of an input parameter. **FOCUS SCENARIO SPECIFIC.** As sorption is taken to be pH independent, pH values are treated as dummy values.
Table horizon VanGenuchtenPar Table specifying the VanGenuchten parameters for each horizon	Specify for each soil horizon: 1) The saturated water content ($m^3.m^{-3}$) [0|0.95], 2) The residual water content ($m^3.m^{-3}$) [0|0.04, 3) Parameter alpha (cm-1) [1.d-3|1], 4) Parameter n (-) [1|5], 5) The saturated conductivity ($m.d^{-1}$) [1.d-4|10], and 6) Parameter lambda (l) (-) [-25|25]. **FOCUS SCENARIO SPECIFIC**
OptRho Option for input of bulk density data	OptRho set to 'Input'. Rho ($kg.m^{-3}$) specified for each horizon. **DEVELOPMENT DEFINITION.**
ZPndMax Maximum thickness of ponding water layer Ponding depth	The default value for the maximum thickness of ponding water layer is used, i.e. 2 mm. When the computed thickness of the ponding water layer exceeds 2 mm, the excess of water will be removed as run-off. **DEVELOPMENT DEFINITION**
FacEvpSol Coefficient for evaporation from bare soil	Set to 1.0. **FOCUS DEFINITION**

CofRedEvp	Soil evaporation coefficient	The coefficient is set at 0.79 $cm^{1/2}$. **DEVELOPMENT DEFINITION**
Table horizon LenDisLiq	Dispersion length of solute in liquid phase [at least 0.5 times the compartment thickness]	Set to 5 cm for all layers. **DEVELOPMENT DEFINITION**
OptCofDifRel	Option for Tortuosity	The option of the relation of Millington & Quirk (1960) is selected. OptCofDifRel set to MillingtonQuirk. **DEVELOPMENT DEFINITION**
ExpDifLiqMilNom	Exponent in nominator of relation of Millington & Quirk for diffusion in the liquid phase.	Set to 2 (-). **DEVELOPMENT DEFINITION**
ExpDifLiqMilDen	Exponent in denominator of relation of Millington & Quirk for diffusion in the liquid phase.	Set to 0.67 (-). **DEVELOPMENT DEFINITION**
ExpDifGasMilNom	Exponent in nominator of relation of Millington & Quirk for diffusion in the gas phase.	Set to 2 (-). **DEVELOPMENT DEFINITION**
ExpDifGasMilDen	Exponent in denominator of relation of Millington & Quirk for diffusion in the gas phase.	Set to 0.67 (-). **DEVELOPMENT DEFINITION**
Section 3: Meteo Section		
MeteoStation	Name of MeteoStation	The name of the station is based on the name of each FOCUS location. **DEVELOPMENT DEFINITION**
OptEvp	Option to select the type of data used by the model.	OptEvp set to Input. Use of reference evapotranspiration (Etref) data. **FOCUS DEFINITION**
Lat	Latitude of the meteo station	Maximum is 60°. **FOCUS SCENARIO SPECIFIC**.
Alt	Altitude of the meteo station (m)	This parameter is not relevant for the FOCUS scenarios, so a dummy value is introduced, i.e. –99. **DEVELOPMENT DEFINITION.**
TemLboSta	Initial lower boundary soil temperature [-20|40]	The initial temperature at the lower boundary is set equal to the average of the maximum and minimum air temperature on the first day of the first simulation year. **DEVELOPMENT DEFINITION.** The upper boundary temperature is read from meteo file. **FOCUS SCENARIO SPECIFIC**
OptIrr	Option to choose between a scenario with and a scenario without irrigation	OptIrr set to no for FOCUS location-crop combinations for which irrigations are not considered. OptIrr set to yes for location-crop combinations for which irrigations are considered. **FOCUS SCENARIO SPECIFIC**

IrrigationScheme Identification of the irrigation scheme	The name consists of a combination of the first four letters of the FOCUS location, the suffix 'IRR' and the suffix specifying the irrigation crop group code, e.g. CHAT-IRR-F. **DEVELOPMENT DEFINITION.**
Section 4: Lower Boundary flux	
ZGrwLevSta Initial depth of groundwater level (m)	The value for the initial groundwater level, is taken to be equal to the average groundwater level for the specified location for which the scenario is run., except for Porto where the initial groundwater level is taken to be equal to the average groundwater level in the winter. Because a sinus function is used to describe the course with time of the groundwater level for Piacenza, the groundwater level calculated for the first day of the year is taken as the initial groundwater level. **DEVELOPMENT DEFINITION.**
In one run the user has to choose between one of the eight lower boundary options that follow below.	In this section the option for the bottom boundary condition is specified.
1. GrwLev Groundwater level data input	Option 'GrwLev' offers the possibility to introduce data on the course with time of the ground water level within the year. In each scenario with this option selected, the course with time of the groundwater level applies to all simulated years. For the Piacenza site, the variation in the groundwater level is limited, it ranges between 0.7 and 1.3 m. The course of the groundwater level in this profile could not be simulated with the option 'FncGrwLev': the resulting fluctuations in the ground water level were far greater than the 0.6 m as given in the description of this profile. Therefore, the OptLbo GrwLev was selected and a sinus function was used to describe the variation in the ground water level. The amplitude was set at 0.3 m and the average groundwater level was set at 1.0 m. Using this function it was assumed that the ground water was deepest on 1 August and shallowest on 1 February. The computed daily values were introduced in the table GrwLev. **FOCUS SCENARIO SPECIFIC**
2. Flux Regional bottom flux	Not used in FOCUS scenarios.
3. Head Flux from deep aquifer	Not used in FOCUS scenarios.
4. FncGrwLev Bottom flux as function of groundwater level	OptLbo FncGrwLev offers the possibility of calculating the water flux at the bottom boundary of the soil system, q (cm d^{-1}), as a function of the groundwater level h (in cm below the surface, negative value). If this option is chosen then the groundwater level should be within the simulated soil profile during the whole simulation period. The function for the description of the bottom flux is given by: $q = A \exp(B \cdot h)$ in which the coefficient A, CofFncGrwLev, must be

		expressed in $m.d^{-1}$ and the coefficient B, ExpFncGrwLev, in m^{-1}. For the Hamburg, Jokioinen, Kremsmünster, Porto and Sevilla sites, the groundwater level was described by setting OptLbo at FncGrwLev. The value of A was –0.01 m d^{-1} for each site. The value of B was estimated by judgement of graphical output from test runs of the course with time of the groundwater table using meteodata for three consecutive years. The computed course was compared with the limited data available on the (average) groundwater level in the soil profile. For the Hamburg, Jokioinen, Kremsmünster, Porto and Sevilla sites the value of B was estimated to be –1.4, -2.0, -1.7, -1.25 and –2.5 m^{-1} respectively (See Figure 1 for examples of groundwater fluctuations). **FOCUS SCENARIO SPECIFIC**
5. Dirichlet	Pressure head of bottom compartment	Not used in FOCUS scenarios.
6. ZeroFlux	Bottom flux equals zero	Not used in FOCUS scenarios.
7. FreeDrain	Free drainage of soil profile	The ground water level for the Châteaudun (around 12 m), Okehampton (around 20 m) and Thiva (> 5 m) sites is deep, so OptLbo is set to FreeDrain which allows free drainage at the bottom of the soil profile. **FOCUS SCENARIO SPECIFIC**
8. Lysimeter interface	Free outflow at soil-air	Not used in FOCUS scenarios.
Section 4b: Drainage/infiltration section		
NumDraLev	Number of drainage levels	NumDraLev set to 0. Drainage not considered in FOCUS scenarios. **FOCUS DEFINITION**
Section 5: Substance section		
MolMas_subst1	Substance Molar Mass	In g/mol. **USER INPUT**
Table compounds Subst1 End_table	List of substances.	First substance is parent, the others are metabolites. **USER INPUT**.
Table FraPrtDau (mol.mol-1) 0.71 Subst1 -> MET- Subst1 end_table		Transformation table (parent-daughter relationships). The fraction transformed is expressed on an amount-of-substance basis (so in $mol.mol^{-1}$). The fractions transformed have to be estimated from soil metabolism studies for transformation products. **USER INPUT**.
OptCntLiqTraRef_subst1	Option to use the moisture content during the incubation study (CntLiqTraRef)	Set to 'OptimumConditions'. Using this option, it is assumed that the incubation experiment has been done under optimum moisture conditions (matric pressure of –100 hPa). **DEVELOPMENT DEFINITION**

DT50Ref_subst1	Half-Life of transformation	DT50 (half-life) in days at reference conditions (topsoil, 20 degrees Celsius and matric pressure of – 100 hPa). **USER INPUT**
TemRefTra_subst1	Temperature of reference at which the half-life of transformation was measured	In Celsius. **USER INPUT**
ExpLiqTra_subst1	Coefficient describing the relation between the transformation rate of the substance and the volume fraction of liquid	**USER INPUT**. Default value defined by FOCUS 0.7 (dimensionless).
CntLiqTraRef_subst1	Reference content of liquid in transformation study from which DT50 was derived	Not used in FOCUS scenarios. **DEVELOPMENT DEFINITION**
MolEntTra_subst1	Molar activation enthalpy of transformation	**USER INPUT**. Parameter in Arrhenius equation describing the relation between the conversion rate of the substance and soil temperature. Default value defined by FOCUS workgroup 54 $kJ.mol^{-1}$.
Table horizon FacZTra	Factor for the influence of depth on transformation rate in soil as a function of soil layer [0|1]	List with length equal to number of horizons. **FOCUS SCENARIO SPECIFIC**
OptCofFre	Option to choose between pH-dependent or pH-independent sorption	Set to pH-independent, so the Freundlich sorption equation is used. The sorption coefficient is calculated by multiplying the coefficient of sorption on organic matter and the organic matter content. **FOCUS DEFINITION.**
ConLiqRef_subst1	Reference liquid content for the sorption coefficient	Set to 1 $mg.L^{-1}$. **DEVELOPMENT DEFINITION**
ExpFre_subst1	Freundlich exponent	**USER INPUT**.
KomEql_subst1	Coefficient of equilibrium sorption of substance on organic matter (Kom).	In L/kg. **USER INPUT**
Gas/liquid partitioning		
PreVapRef_subst1	Saturated vapour pressure of substance	In Pa. Measured at temperature TemRefVap. **USER INPUT**
TemRefVap_subst1	Temperature of reference at which the saturated vapour pressure was measured	In degrees Celsius. **USER INPUT**
SlbWatRef_subst1	Water solubility of substance	Mass concentration in water at saturation (in mg/L) measured at reference temperature TemRefSlb. **USER INPUT**
TemRefSlb_subst1	Temperature of reference at which the water solubility was	In degrees Celsius. **USER INPUT**

	measured	
MolEntSlb_subst1	Molar enthalpy of the dissolution	**USER INPUT**. Describing the relation between the water solubility of the substance and temperature. Default value defined by FOCUS workgroup 27 kJ/mol.
MolEntVap_subst1	Molar enthalpy of the vaporization process	**USER INPUT**. Describing the relation between the saturated vapour pressure of the substance and temperature. Default value defined by FOCUS workgroup 95 kJ/mol.
Non-equilibrium sorption		
CofDesRat_subst1 FacSorNeqEql_subst1	Rate of desorption Factor relating coefficient for equilibrium and non-equilibrium sorption	Non-equilibrium sorption not considered in FOCUS scenarios, so CofDesRat_subst1 and FacSorNeqEql_subst1 are set to zero. **FOCUS DEFINITION**
Uptake		
FacUpt_subst1	Coefficient for uptake by plant roots	**USER INPUT**. Passive uptake due to transpiration (dimensionless). Default value defined by FOCUS workgroup Set to 0.5.
Volatilization		
ThiAirBouLay	Thickness of the stagnant air layer at the soil surface	Set to 0.01 m. **DEVELOPMENT DEFINITION**
Canopy processes		
OptDspCrp	Option for the description of the loss routes of substance from the crop surface	Option set to ‘Lumped’. In the FOCUS scenarios only soil applications occur, so these parameters are not relevant. **DEVELOPMENT DEFINITION**
DT50DspCrp	Half-life for the disappearance of the substance on the crop	If OptDspCrp is set to ‘Lumped’ then value for DT50DspCrp (d) is required. Because no crop applications occur in the FOCUS scenarios, this value is considered as a dummy value. **DEVELOPMENT DEFINITION**
FacWasCrp	Factor for the wash-off of substance from the crop by rainfall or irrigation.	Not relevant in FOCUS scenarios. **DEVELOPMENT DEFINITION**
Diffusion of solute in liquid and gas phases		
TemRefDif_subst1	Temperature of reference at which diffusion coefficients were measured	In degrees Celsius. **USER INPUT**
CofDifWatRef_subst1	Coefficient of diffusion of the substance in water	**USER INPUT**. Default value defined by FOCUS workgroup 4.3E-5 m^2/d.
CofDifAirRef_subst1	Coefficient of diffusion of the substance in air	**USER INPUT**. Default value defined by FOCUS workgroup 0.43 m^2/d.
Section 6: Management section		
Application-Scheme	Name of application scheme.	**USER INPUT**.
ZFoc	FOCUS target depth (m)	Set to 1.0 m. **USER INPUT.**

DelTimEvt	Time difference in years between two subsequent events	For the 26-years, 46-years, and 66-years scenarios DelTimEvt is set to 1, 2 and 3 respectively. **DEVELOPMENT DEFINITION**
Management events table Applications 01-Emg-01 AppSolSur 1.00 end_table		The first two columns of the Applications table contain: 1) The application dates and 2) The application option. The application dates can be relative to the day of emergence(Emg) or the day of the harvest (Har) or they can be specified as dates. In the FOCUS scenarios the application option is always set to AppSolSur: application at the soil surface. When the application option is set to AppSolSur then column 3 contains the dosage (kg/ha).
table TillageDates end_table	Date and depth of tillage for each tillage event.	No ploughing is considered, so no dates are entered. **FOCUS DEFINITION**.
Initial conditions Table interpolate CntSysEql z B 0.00 0.00 50.0 0.00 end_table	Concentration in equilibrium domain	In mg.kg^{-1}. Concentration set to 0. **FOCUS DEFINITION**.
Table interpolate CntSysNeq B 0.00 0.00 50.0 0.00 end_table	Concentration in non-equilibrium domain	In mg.kg^{-1}. Concentration set to 0. **FOCUS DEFINITION**.
Upper boundary flux table FlmDep end_table	Date and flux of deposition (kg.ha-1.da-1)	No dates are entered, so the flux is zero throughout the simulation period. **FOCUS DEFINITION**.
Section 7: Crop section		
RepeatCrops	Option to repeat the growth of the same crop each year	Set to 'Yes'. **FOCUS DEFINITION**.
Table Crops 20-Sep-1901 15-Aug-1901 Sugarbeet end_table	Crop calendar table	The table contains three columns: 1) emergence date, 2) harvest date and 3) name of the crop. For the FOCUS scenarios RepeatCrops is set to 'Yes', so the specification of the year is not required. Crop dates are specified according to the data specified for the crops in the FOCUS scenarios. **FOCUS SCENARIO SPECIFIC**
OptLenCrp	Option to select the type of plant growth model	Set to 'Fixed', so the length of the crop cycle fixed is the same each year. **DEVELOPMENT DEFINITION**
Table CrpPar_sugarbeet 0.00 0.00 1.00 0.00 0.00 0.72 0.10 1.00 0.20 0.00	Table with crop parameters	Table with crop parameters as a function of development stage. The table contains 5 columns: 1) the development stage (development stage at

0.84 4.80 0.74 0.95 0.00 1.00 4.80 0.74 0.95 0.00 end_table	emergence = 0; development stage at harvest =1) , 2) LAI: Leaf Area Index (m2.m-2), 3) Crop factor for evaporation, 4) Rooting depth (m) and 5) Crop height (m). In the input data for the FOCUS scenarios, the LAI is given as a function of the Julian day number. Three time points are given, i.e. the day of emergence (or leaf emergence), the day when the maximum LAI is reached and the day of the harvest (or leaf fall). For the first and the last time point the value for the DVS is known. Because the DVS is a linear function of time, the value for the DVS on the day when the maximum LAI is reached is calculated from the Julian day number by linear interpolation. Thus, the LAI is a linear function of time based on three pairs of DVS-LAI values. Note that the day on which the maximum LAI is reached is always the same, so the value for the DVS when the maximum LAI is reached is also the same each year. For winter crops, an additional DVS-LAI pair is introduced. It is assumed that little growth occurs during the winter period. Therefore, real crop growth is assumed to start as soon as the average daily temperature reaches 10 °C. On this day the LAI is taken to be 0.1. For winter oil seed rape growth starts as soon as the temperature reaches 7.5 °C. The values for the crop factor for evaporation are specified by the FOCUS workgroup and these data were transformed into DVS-CF pairs using the same procedure as for the LAI. The values for the rooting depth are defined as a function of time by the FOCUS workgroup and these data were transformed into DVS-RDTB pairs using the same procedure as for the LAI. For perennial crops the rooting depth is constant throughout the year. **FOCUS SCENARIO SPECIFIC** Because crop height is not relevant in the FOCUS project, dummy values are used. **DEVELOPMENT DEFINITION**
Table RootDensity_ sugarbeet Root density table 0.00 1.00 1.00 1.00 end_table	The root density table contains two columns: 1) the relative rooting depth (0 at soil surface and 1 the rooting depth) and 2) the relative root density (-). The root density distribution is listed as a function of the relative rooting depth. The default values of SWAP are taken, so the potential rate of water uptake is uniform over the rooting depth. **DEVELOPMENT DEFINITION**
Crop water use HLim1_ sugarbeet no water extraction at higher pressure heads HLim2_ sugarbeet pressure head below which optimal water use HLim3U_ sugarbeet pressure head below which reduction starts when Tpot high HLim3L_ sugarbeet pressure head below which reduction starts when Tpot low HLim4_ sugarbeet No water extraction below this pressure	For the description of the crop water use, values for the parameters in the water extraction function (all in cm water pressure) of Feddes et al. (1978) are specified for each crop (See Van Dam et al., 1997). For the crops in the FOCUS scenarios the values for the parameters in the water extraction function are listed in Table 1. **DEVELOPMENT DEFINITION**
RstEvpCrp_ sugarbeet Canopy resistance	Because the Penman-Monteith equation is not used in the FOCUS scenarios, the value for the minimum

		canopy resistance (RstEvpCrp, in s.m^{-1}) is treated as a dummy. **DEVELOPMENT DEFINITION**
CofExtRad_ sugarbeet	Extinction coefficient for global radiation	CofExtRad equals 0.39, i.e. the same value as that specified by Ritchie (1972) and Feddes (1978). **DEVELOPMENT DEFINITION**
CofIntCrp_ sugarbeet	Interception coefficient	In the FOCUS scenarios, the interception of water by the crop is assumed to be negligible. The value for the coefficient of Von Hoyningen-Hune and Braden, is set at 0. **FOCUS DEFINITION**
TemSumSta_ sugarbeet	Start value of temperature sum	Not considered in FOCUS scenarios. Treated as a dummy. **DEVELOPMENT DEFINITION**
TemSumEmgAnt_ sugarbeet	Temperature sum from emergence to anthesis	Not considered in FOCUS scenarios. Treated as a dummy. **DEVELOPMENT DEFINITION**
TemSumAntMat_ sugarbeet	Temperature sum from anthesis to maturity	Not considered in FOCUS scenarios. Treated as a dummy. **DEVELOPMENT DEFINITION**

Y.IRR file

Parameter and description		Value, source & comments
Table IrrTab	Table with irrigation table	The irrigation table contains two columns: 1) the date of irrigation in the format day-month-year and 2) the depth of the irrigation water layer (mm). The irrigation data for scenarios with irrigation are those prepared by the FOCUS workgroup. **FOCUS SCENARIO SPECIFIC**

Y.MET file

Parameter and description		Value, source & comments
Meteo table data	Table with meteorological	The meteo data are extracted from the MARS dataset for all locations. The meteo data file contains daily data in 11 columns: 1) the name of the weather station, 2) the day, 3) the month, 4) the year, 5) the solar radiation (kJ m^{-2}), 6) the minimum air temperature (°C), 7) the maximum air temperature (°C), 8) the air humidity (kPa), 9) the wind speed (m s^{-1}), 10) the rainfall (mm) and 11) the reference evapotranspiration (mm). **FOCUS SCENARIO SPECIFIC**

Table 1 Values for coefficients (in cm water layer)[a] in the water withdrawal function based on Feddes et al. (1978) for the crops selected by the FOCUS workgroup.

Crop	HLIM1	HLIM2U	HLIM2L	HLIM3H	HLIM3L	HLIM4
Apples	-10.0	-25.0	-25.0	-500.0	-800.0	-16000.0
Bush berries	-10.0	-25.0	-25.0	-200.0	-300.0	-16000.0
Cabbage	-10.0	-25.0	-25.0	-600.0	-700.0	-16000.0
Carrots	-10.0	-25.0	-25.0	-550.0	-650.0	-16000.0
Citrus	-10.0	-25.0	-25.0	-300.0	-700.0	-16000.0
Cotton	-100.0	-100.0	-100.0	-1000.0	-2000.0	-16000.0
Field Beans	-10.0	-25.0	-25.0	-750.0	-2000.0	-16000.0
Grass	-10.0	-25.0	-25.0	-200.0	-800.0	-8000.0
Linseed	-0.0	-1.0	-1.0	-500.0	-900.0	-16000.0
Maize	-15.0	-30.0	-30.0	-325.0	-600.0	-8000.0
Onions	-10.0	-25.0	-25.0	-500.0	-600.0	-16000.0
Peas	-10.0	-25.0	-25.0	-300.0	-500.0	-16000.0
Soybean	-10.0	-25.0	-25.0	-750.0	-2000.0	-16000.0
Summer cereals	-0.0	-1.0	-1.0	-500.0	-900.0	-16000.0
Summer oil seed	-0.0	-1.0	-1.0	-500.0	-900.0	-16000.0
Summer potatoes	-10.0	-25.0	-25.0	-320.0	-600.0	-16000.0
Sunflower	-15.0	-30.0	-30.0	-325.0	-600.0	-8000.0
Strawberries	-10.0	-25.0	-25.0	-200.0	-300.0	-16000.0
Sugarbeet	-10.0	-25.0	-25.0	-320.0	-600.0	-16000.0
Tobacco	-10.0	-25.0	-25.0	-300.0	-800.0	-16000.0
Tomatoes	-10.0	-25.0	-25.0	-800.0	-1500.0	-16000.0
Vegetable beans	-10.0	-25.0	-25.0	-750.0	-2000.0	-16000.0
Vines	-10.0	-25.0	-25.0	-700.0	-750.0	-16000.0
Winter cereals	-0.0	-1.0	-1.0	-500.0	-900.0	-16000.0
Winter oil seed	-0.0	-1.0	-1.0	-500.0	-900.0	-16000.0

[a)] HLIM1 = pressure head above which there is no water extraction; HLIM2U = pressure head below which optimal water extraction starts for top layer; HLIM2L = pressure head below which optimal water extraction starts for soil sub-layer; HLIM3H = pressure head below which reduction in water extraction starts if potential transpiration is high; HLIM3L = pressure head below which reduction in water extraction starts if potential transpiration is low; HLIM4 = pressure head below which there is no water extraction.

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