Project no. 022704 (SSP)

FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

Specific Targeted Research Project

Thematic Priority: Policy-orientated research

Deliverable DL20

Database containing complete PRZM parameterisation for FOOTPRINT soil, climate and crop scenarios

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Dissemination Level		
PU	Public	**X**
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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Foreword

The present report was prepared within the context of the work package WP4 ("Parameterisation, meta-modelling and risk assessment") of the FOOTPRINT project (http://www.eu-footprint.org).

The preferred reference to the present document is as follows:
Reichenberger S., Dubus I.G., Boulahya F., Hollis J.M. & Jarvis N.J. (2008). Database containing complete PRZM parameterisation for FOOTPRINT soil, climate and crop scenarios. Report DL20 of the FP6 EU-funded FOOTPRINT project [www.eu-footprint.org], 32p.

Executive summary

PRZM is a one-dimensional pesticide fate model which is able to simulate pesticide losses from fields via surface runoff and erosion. PRZM is used in FOOTPRINT to make EU-wide predictions of pesticide inputs into surface waters via surface runoff and erosion.

The first part of the FOOTPRINT work consisted in addressing an issue related to the parameterisation of PRZM. PRZM uses the SCS Curve Number approach for the calculation of surface runoff. The SCS Curve Number Approach calculates stream response to heavy rainfall events and thus implicitly includes all components of fast flow to surface water: infiltration excess runoff, saturation excess runoff, lateral subsurface flow, channel runoff and, where applicable, drainflow. Although PRZM is based on the SCS Curve Number, it implements it in an inadequate way as all water flow is considered to originate from infiltration excess runoff. We therefore adjusted the USDA soil hydrologic groups (which determine the curve numbers and thus the frequency and magnitude of runoff events) so that they only reflect surface runoff (infiltration excess runoff + saturation excess runoff). Lateral subsurface flow is calculated in FOOTPRINT with the model MACRO.

Several data sources were used to support the calculation of PRZM input parameters: the Soil Geographic Database of Europe, v. 1.0 was used to identify 264 ‘benchmark’ soil profiles (‘FOOTPRINT soil types’) which characterise agricultural land in Europe. The following data, which are available in the SPADE-2 database for soil horizons, were used to support the parameterization of hydraulic properties in the model: horizon designation; upper depth; lower depth; clay, silt and sand; stone content; pH; organic carbon content; bulk density. Each soil type is classified into one of 15 unique hydrological classes based on the HOST (‘Hydrology of Soil Types’) system, the FOOTPRINT hydrologic groups (FHG). These determine the USDA hydrologic group and thus the curve numbers. For parameters other than basic soil property data and soil hydrologic group, PRZM was parameterised using both the parameterisation guidance in the PRZM 3.12.1 manual (Carsel et al., 2003) and in the FOCUS surface water report (FOCUS, 2001). Crop parameters were harmonized with the crop parameters used in MACRO within FOOTPRINT.

Finally, the parameterisation, running and postprocessing tasks of PRZM were fully automated to enable a large number of modelling runs to be undertaken.

1 INTRODUCTION

This report presents the results of work carried out within the FOOTPRINT project to develop a consistent and complete set of parameter estimation routines for the PRZM model (Carsel et al., 2003) to allow EU-wide simulations of pesticide losses from fields via surface runoff and erosion based on only readily available data (e.g. soil survey data and soil profile descriptions). The system is compatible with the data available at the EU level, and also those which farmers and extension advisors could gather quickly and at reasonable cost at the local field and farm scales.

PRZM (**P**esticide **R**oot **Z**one **M**odel) is a one-dimensional, dynamic, compartmental finite-difference model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the root zone (Carsel et al., 2003). The original version of the PRZM model was released in 1984 (Carsel et al., 1984). The model has been continuously improved since then. The latest, Windows-based version PRZM 3.21β is used in the context of the FOCUS surface water scenarios (FOCUS, 2001) as runoff and erosion model. A version with only minor differences is also used as one of the official leaching models in the FOCUS groundwater scenarios (FOCUS, 2000).

The PRZM model is able to simulate surface runoff, erosion, leaching, decay, plant uptake, foliar washoff, and volatilisation of pesticides. It has two major components – water and chemical transport. The processes of PRZM relevant for runoff and erosion modelling are described in the model as follows:

1.1 Water Transport

PRZM is a capacity-type model with a daily time step. Water movement is simulated with a rather simple approach. The soil profile is divided into several layers. A soil layer is characterized by three hydraulic parameters: field capacity (usually reported as the amount of water the soil can hold against the influence of gravity), wilting point (the soil moisture content below which plants can no longer extract water from the soil), and saturated water content (pore volume). If the soil water content of a soil layer exceeds field capacity, the excess water drains to the next layer. The whole soil profile drains within one day to field capacity. Thus, PRZM is not able to simulate waterlogging. As PRZM is also unable to simulate preferential flow, its application should be restricted to well-drained soils without strongly developed soil structure if leaching estimates are required. However, since waterlogging rarely occurs in the topsoil and leaching by preferential flow does not significantly affect bulk pesticide concentrations in the topsoil, these limitations do not affect the general applicability of PRZM to runoff and erosion problems.

Evapotranspiration in PRZM is composed of evaporation from crop interception, evaporation from soil and transpiration from the crop. Potential evapotranspiration is obtained from direct input of daily pan evaporation, multiplied with a crop-specific correction factor.

PRZM is not able to simulate upward water movement due to hydraulic potential gradients induced by evapotranspiration. This can lead to an underestimation of actual evapotranspiration.

Surface runoff is described by a modification of the empirical USDA Soil Conservation Service (SCS) Curve Number technique (Haith and Loehr, 1979):

$$Q = \frac{(P + SM - 0.2S)^2}{P + SM + 0.8S} \quad \text{for } (P + SM - 0.2\,S) > 0 \qquad \text{(eq. 1)}$$

$$Q = 0 \quad \text{for } (P + SM - 0.2\,S) \le 0$$

where

Q surface runoff (cm d^{-1})

P precipitation as rainfall, minus crop interception (cm d^{-1})

SM snowmelt (cm d^{-1})

S daily watershed retention parameter (cm d^{-1}); 0.2 S is also referred to as “initial abstraction”

The daily watershed retention parameter *S* is estimated by

$$S = \frac{1000}{CN} - 10 \qquad \text{(eq. 2)}$$

with

CN SCS runoff curve number ($0 < CN \le 100$)

Curve numbers are a function of soil type, soil drainage properties, crop type and management practice (Carsel et al., 2003). The higher the curve number, the more frequently runoff will occur, and the higher the runoff volume per event will be. In PRZM, the curve numbers are adjusted daily as a function of the soil water status in the upper soil layers, following the algorithms developed and reported by Haith and Loehr (1979). Runoff curve numbers are tabulated for different crops and soil hydrologic groups in the PRZM 3.12.1

Manual (Carsel et al., 2003). Curve numbers and thus runoff susceptibility increase from group A (light, sandy soils) to D (heavy, clayey soils). Note that although PRZM considers the effect of snowmelt in the runoff equation, the curve numbers are not adjusted to account for the effects of snowpack or frozen ground on runoff generation.

Soil loss by sheet and rill erosion is also modelled empirically using the Modified Universal Soil Loss Equation (MUSLE; Williams, 1975) or one of its modifications (MUSS, MUST). MUSS was specifically designed for small watersheds and is used in the PRZM calculations in the FOCUS surface water scenarios.

$$\text{MUSLE: } X_e = 1.586\,(V_r\,q_p)^{0.56}\,A^{0.12}\,K\,LS\,C\,P \qquad \text{(eq. 3)}$$

$$\text{MUSS: } X_e = 0.79\,(V_r\,q_p)^{0.65}\,A^{\,0.009}\,K\,LS\,C\,P \qquad \text{(eq. 4)}$$

where

X_e	event soil loss (t d^{-1})
V_r	volume of event (daily) runoff (mm)
q_p	peak storm runoff rate (mm h^{-1})
A	field size (ha)
K	soil erodibility factor (dimensionless)
LS	length-slope factor (dimensionless)
C	soil cover factor = crop management factor (dimensionless)
P	conservation practice factor (dimensionless)

While *A*, *K*, *LS*, *C* and *P* are user input, q_p is calculated internally in PRZM, using a generic storm hydrograph. The rainfall intensity is assumed to occur according to “design storm distributions” or rainfall regimes. The rainfall regime is entered by the PRZM user. For Western and Middle Europe, type II, which covers the largest part of the USA without the Atlantic, Pacific and southern regions, is the most appropriate rainfall regime.

1.2 Pesticide Transport and Fate

In contrast to the older PRZM version 3.12 used by the US Environmental Protection Agency (USEPA), the latest version 3.21β is also capable of modelling non-linear sorption and temperature- and moisture-dependent degradation (FOCUS, 2001). Sorption is described identically as in MACRO using a Freundlich isotherm (eq. 3.11, section 3.1.2). Degradation is by default described by single first-order kinetics; however, there is also a possibility to specify biphasic degradation with a “hockey-stick” model, which switches from a fast first-order kinetic to a slower one at a user-defined time point.

The temperature dependence of degradation is based on a Q_{10} equation, which is mathematically equivalent to the formula used in MACRO (cf. eq. 3.16, section 3.1.2) as an approximation of the Arrhenius equation. The moisture-dependence of degradation is described in PRZM with the Walker formula (eq. 3.15, section 3.1.2). However, in PRZM the reference moisture can be freely chosen, either as absolute volumetric moisture or in percent of field capacity.

The extraction of pesticides from soil with runoff water follows an empirical approach, where the runoff-availability of a compound decreases with depth (“non-uniform extraction model”; Carsel et al., 2003):

$$DRI_i = 0.7 \cdot \left(\frac{1}{2.0 \cdot Midtot_i + 0.9} \right)^2 \qquad \text{(eq. 5)}$$

where

DRI_i	fraction of dissolved-phase chemical present in compartment i available for runoff (dimensionless)
$Midtot_i$	depth to midpoint of compartment i (cm)
0.7	efficiency factor
0.9	depth-reduction coefficient

Calculations are performed for all compartments *i* from the surface to a depth of 2 cm; the thickness of the topsoil compartments is usually set to 0.1 cm. Thus, the runoff-available fraction decreases from 70 % of the dissolved chemical in the uppermost compartment to 3 % in the 20th compartment. Below 2 cm depth the runoff availability of chemicals is zero. Pesticide runoff loss from compartment *i* is then obtained as

$$J_{r,i} = DRI_i \cdot C_i \cdot Q \cdot 10 \qquad \text{(eq. 6)}$$

with

$J_{r,i}$	pesticide runoff loss from compartment i (mg m^{-2} d^{-1})
C_i	concentration of dissolved pesticide in the water phase (mg L^{-1})
10	unit correction factor

During erosion events, apart from losses dissolved in surface runoff, pesticides can also leave the field adsorbed to eroded topsoil material. Because erosion is a selective process, eroded soil material is, compared with the topsoil from which it was eroded, enriched in smaller particles and organic matter (the main sorbent for non-ionic pesticides). In PRZM, the enrichment ratio for organic matter r_{om} is calculated empirically according to the following equation:

$$\ln (r_{om}) = 2 - 0.2 \ln (1000\, X_e/A) \qquad \text{(eq. 7)}$$

Thus, larger erosion events are less selective and will result in lesser enrichment of organic matter. Pesticide loss from the field via erosion is calculated as

$$J_e = \frac{X_e \cdot r_{om} \cdot S_1}{10 \cdot A} \qquad \text{(eq. 8)}$$

with

J_e	pesticide erosion loss (mg m^{-2} d^{-1})
S_1	concentration of adsorbed pesticide in the solid phase (mg kg^{-1}) in the uppermost compartment
10	unit correction factor

In contrast to MACRO, PRZM is also able to model pesticide losses via volatilization. PRZM explicitly simulates vapour phase diffusion in soil, volatilization from soil and plant surfaces, and volatilization flux through the plant canopy. A detailed process description cannot be given here, but can be found in Carsel et al. (2003). Pesticide washoff from the crop canopy to the soil surface is modelled using an empirical extraction coefficient Pesticide uptake by roots is treated in the same way as in MACRO as a passive process with a plant uptake concentration factor between 0 and 1.

2 PARAMETERISATION OF PRZM

The rules used to parameterise the PRZM model are outlined in the table below.

Record	Parameter name	Description	FOOTRINT parameterisation
1	TITLE	Label for simulation title	Set to the FOOTPRINT Unique Numbering. Uniquely identifies each of the FOOTPRINT model runs
2	HTITLE	Label for hydrology information title	N/A
3	PFAC	Pan factor used to estimate daily evapotranspiration	Set to 1 since PET is fed directly.
3	SFAC	Snowmelt factor in cm/°C	Set to 0.46 (default value from FOCUSgw)
3	IPEIND	Pan factor flag	Set to 0 (pan data read)
3	ANETD	Minimum depth of which evapotranspiration is extracted (cm); the value of ANETD applies when the soil is bare and only evaporation can	Depending on climate zone; Rules used: (arbitrary, following FOCUS) annual Tmean ANETD < 5 °C 10 5 - < 9.5 °C 15 9.5 - > 13 °C 20 13 - < 16 °C 25 >= 16 °C 30

		occur	Results: FCZ ANETD 1 20 2 20 3 15 4 10 5 20 6 15 7 20 8 30 9 30 10 10 11 25 12 15 14 15 15 15 16 15
3	INICRP	Indicates the initial crop if the simulation start date occurs before the emergence date of the first crop	1 (in theory, only used if erosion is switched off; however, if INICRP is set to zero, PRZM operates wrongly)
3	ISCOND	Surface condition of initial crop	1 (in theory, only used if erosion is switched off; set according to FOCUSsw)
6	ERFLAG	Flag to calculate erosion	Set to 4 in accordance with FOCUSsw (MUSS approach)
7	USLEK	soil erodibility factor K of the	Calculated for each of the 264 FSTs. The PRZM 3.12.1 Manual (Carsel et al., 2003) lists values of USLEK for different combinations of USDA texture class

		Universal Soil Loss Equation (USLE) and its modifications (MUSLE/MUSS)	and 3 levels of OM content (< 0.5, 2 and 4 %). Unfortunately, the manual doesn't give class boundaries; hence we set the class boundaries to 1 % and 3 % OM, yielding three classes: 0 - < 1 % OM, 1 - < 3 % OM, >= 3 % OM. For each FST, the USDA texture class and the OM class of the uppermost horizon were determined. Subsequently, the USLEK value for the respective texture class / OM class combination was assigned to each FST. USLEK values for FSTs with organic topsoils were set to 0.01 (topsoil with 50 % OC) and 0.02 (topsoil with 26 % OC).
7	USLELS	Topographic factor LS of the USLE (combined slope length / steepness factor)	Calculated according to the SWAT2005 Theory (Neitsch et al., 2005) with the following formula: $USLELS = (L_{hill}/22.1)^m * (65.41 * \sin^2 (\alpha_{hill}) + 4.56 \sin (\alpha_{hill}) + 0.065)$ *where* L_{hill} is the slope length (m); set to 100 m in FOOTPRINT α_{hill} is the angle of the slope (rad); set specifically for each FST The exponent m is calculated as follows: $m = 0.6 (1 – \exp(-25.835 * slp))$ *where* slp is the slope expressed as a fraction ($slp = \tan \alpha_{hill}$)
7	USLEP	Erosion control practice factor of the USLE	Calculated FST-specifically according to the PRZM 3.12.1 Manual (Carsel et al., 2003). Contouring is assumed. FST slope (%) — USLEP 0 - 2 — 0.6 > 2 - 7 — 0.5 > 7 – 12 — 0.6 > 12 — 0.8
7	AFIELD	Field area (ha)	Set to 1
7	IREG	Type of rainfall intensity distribution	Different values specified for each of the 16 FCZ. PRZM does not allow to specify intensity distributions directly. One can only choose between different rainfall intensity regimes.

The different IREG in PRZM denote the following:

IREG	occurrence in US	distributions assigned: summer (01/05 - 15/09)	distributions assigned: winter (16/09 - 30/04)
1	Southern California, Alaska, Hawaii	Type I	Type I A
2	NW coast	Type I A	Type I A
3	rest of US	Type II	Type I A; for events > 5.08 cm/d Type I is used
4	Gulf region, Florida, east coast	Type III	Type I A; for events > 5.08 cm/d Type I is used

IREG	Interpretation	suitable for which European regions
1	intermediate intensity in summer, low intensity in winter	Transitional climates
2	Always low intensity	Northern + Western Europe
3	high intensity in summer, low and (for larger events) intermediate in winter	Central Europe + Mediterranean
4	rather high intensity in summer, low and (for larger events) intermediate in winter	no such climate (subtropical east-coast) in Europe

As a result, IREG was assigned to each FCZ as follows:

FCZ	IREG
1	3
2	1
3	3
4	2
5	1
6	3
7	2
8	3
9	3
10	2
11	2
12	2
14	3
15	1
16	2

7	SLP	Land slope (%)	Different values specified for each of the 264 FSTs. First, descriptive statistics (mean, median, min, max etc.) on slopes from a European slope map (provided by O. Cerdan, BRGM) were calculated for each Soil Map Unit (SMU) in the SGDBE. These statistics were used by John Hollis to derive a 'best estimate' average slope for each FST with an arable or permanent crop land use (as indicated by the USE1 & USE2 attributes in the STU.dbf file of the SGDBE).In most cases the estimated slopes were based on the calculated median slope and 'majority' slope of the SMU in which the FST occurs. However, the estimated slopes were adjusted using a 'weighting' parameter based on the fraction of cover of the STU within the SMU multiplied by the calculated area of each SMU used to derive the slope statistics. In a significant number of cases though, the FST did not represent a significant enough fraction of the SMU area used to calculate the slope data for the slope statistics to be relevant. In such cases the slope was estimated either using expert judgement based on the range of soils within the SMU and the calculated slope statistics, or by using the data on slope ranges (SLOPE1 & SLOPE2) given in STU.dbf file of the SGDBE.
7	HL	Hydraulic length (m)	Denotes the length from the most distant point of the field to the field outlet. Assuming a square field of 1 ha area with the outlet in the middle of the lower field boundary yields a hydraulic length of 111.8 m.
8	NDC	Number of different crops in the simulation	Set to 1 (no crop rotation).
9	ICNCN	Crop number of the different crop	Set to 1 (there is only one crop)
9	CINTCP	Maximum interception storage of the crop (cm)	Set specifically for each FOOTPRINT crop (FCR) in accordance with the MACRO parameterization. The corresponding MACRO parameter is CANCAP (mm).
9	AMXDR	Maximum rooting depth of the crop	Set specifically for each combination of FOOTPRINT crop (FCR) and FOOTPRINT soil type (FST) in accordance with the MACRO parameterization. The corresponding MACRO parameters are ROOTMAX (annual crops, m) and

		(cm)	ROOTDEP (perennial crops, m). AMXDR is computed as the minimum of the crop-inherent maximum rooting depth and the depth to the uppermost root-limiting horizon in the soil profile. The rules for determining whether a horizon is root-limiting or not are: 1. the topsoil horizon (number 1) can never be limiting to root growth, regardless of its properties 2. a subsoil horizon must be at least 25 cm thick if it is to restrict root growth
9	COVMAX	Maximum areic coverage of the canopy (%)	3. one or more of the following criteria must be fulfilled: - horizon designation C or R - pH (H_2O) <= 4.5 - sand% > (85 - silt% * 0.5) AND OC content <= 0.2 % - volumetric stone content > 20 % - structure class * = I AND bulk density > 1.65 g cm^{-3} (* for structure classes cf. DL21)
9	ICNAH	Surface condition of the crop after harvest date	Set to 3 (= residue) in accordance with FOCUSsw. This parameter is allegedly only used when erosion is switched off.
9	CN1		Set to 0 (only used if erosion is switched off → not used here)
9	CN2		Set to 0 (only used if erosion is switched off → not used here)
9	CN3		Set to 0 (only used if erosion is switched off → not used here)
9	WFMAX		Set to 0 (only used if CAM = 3 → not used here)
9	HTMAX	Max. canopy height at maturation date (cm)	Set specifically for each FOOTPRINT crop. Derived from FOCUSsw PRZM and MACRO parameterization of crop height (they considerably differ from each other!) and expert judgement.
9A	CROPNO	Crop number	Set to 1 (there is only one crop)
9A	NUSLEC	Number of	Set to 6 (the 4 cropping dates in FOCUSsw turned out too few, because in FOCUSsw the curve number decreases sharply at emergence date from the value for fallow to the value for a fully developed crop).

<table>
<tr><td></td><td></td><td>USLEC factors (and CN and cropping dates)</td><td></td></tr>
<tr><td>9B</td><td>GDUSLEC</td><td>Day to start USLEC, MNGN and CN. The first date has to be the crop emergence date.</td><td>Set specifically for each combination of FCR and FCZ. Since NUSLEC = 6, 6 values for GDUSLEC are required. The 6 crop dates denote the following:
GDUSLEC/GMUSLEC 1 corresponds to emergence
GDUSLEC/GMUSLEC 2 corresponds to ZDATEMIN in MACRO (the point where the crop development becomes faster, matters for winter crops)
GDUSLEC/GMUSLEC 3 corresponds to intermediate development (e.g. half of maximum ground cover)
GDUSLEC/GMUSLEC 4 corresponds to maturity
GDUSLEC/GMUSLEC 5 corresponds to harvest
GDUSLEC/GMUSLEC 6 corresponds to removal of residues
Values were obtained using NUTS2-specific cropping dates collected by all FOOTPRINT partners.</td></tr>
<tr><td>9B</td><td>GMUSLEC</td><td>Month to start USLEC, MNGN and CN. The first date has to be the crop emergence date.</td><td>Set specifically for each combination of FCR and FCZ. Since NUSLEC = 6, 6 values for GDUSLEC are required. The 6 crop dates denote the following:
GDUSLEC/GMUSLEC 1 corresponds to emergence
GDUSLEC/GMUSLEC 2 corresponds to ZDATEMIN in MACRO (the point where the crop development becomes faster, matters for winter crops)
GDUSLEC/GMUSLEC 3 corresponds to intermediate development (e.g. half of maximum ground cover)
GDUSLEC/GMUSLEC 4 corresponds to maturity
GDUSLEC/GMUSLEC 5 corresponds to harvest
GDUSLEC/GMUSLEC 6 corresponds to removal of residues
Values were obtained using NUTS2-specific cropping dates collected by all FOOTPRINT partners.</td></tr>
<tr><td>9C</td><td>USLEC</td><td>Cover management factors C of the USLE for the different crop stages</td><td>Set specifically for each FOOTPRINT crop. Since NUSLEC = 6, 6 values for USLEC are required. The USLEC were set as follows:
<table>
<tr><th>crop type</th><th>USLEC1</th><th>USLEC2</th><th>USLEC3</th><th>USLEC4</th><th>USLEC5</th><th>USLEC6</th></tr>
<tr><td>grass/greenfodder</td><td>0.02</td><td>0.02</td><td>0.02</td><td>0.02</td><td>0.02</td><td>0.02</td></tr>
<tr><td>other permanent crops</td><td>0.2</td><td>0.2</td><td>0.2</td><td>0.2</td><td>0.2</td><td>0.2</td></tr>
<tr><td>annual crops</td><td>0.6</td><td>0.4</td><td>0.3</td><td>0.2</td><td>0.4</td><td>0.9</td></tr>
</table></td></tr>
</table>

9D	MNGN	Manning's roughness coefficient for the different crop stages (apparently unitless)	Set constant to 0.10, in accordance with FOCUSsw.
9E	CN	SCS runoff curve numbers (for antecedent moisture condition II) for the different crop stages	Set specifically for each combination of PRZM soil hydrologic group, FCR and crop stage. The set of Curve Numbers was obtained in 3 steps: 1. The PRZM soil hydrologic group (A, B, B-C, C, D) is determined by the FOOTPRINT hydrologic group. Hence, each FST has a PRZM soil hydrologic group attached to it. PRZM soil hydrologic groups have been adjusted this way that PRZM only calculates surface runoff (while the CN approach originally calculates total direct runoff). 2. The PRZM 3.12.1 Manual lists curve numbers for different PRZM soil hydrologic groups and different combinations of crop group (the CN are for a fully developed crop), agricultural practice and hydrologic condition (e.g. “small grain, contoured, good” and. Each FCR was assigned one of these combinations. → set of curve numbers for each combination of FST and FCR, for fully developed crop and fallow condition. 3. Linear interpolation of CN for the other crop stages according to the following equations: CN1 = CN_fallow - 0.25 (CN_fallow - CN_crop) = 0.75 CN_fallow + 0.25 CN_crop CN2 = CN_fallow - 0.5 (CN_fallow - CN_crop) = 0.5 CN_fallow + 0.5 CN_crop CN3 = CN_fallow - 0.75 (CN_fallow - CN_crop) = 0.25 CN_fallow + 0.75 CN_crop CN4 = CN_crop CN5 = CN_fallow - 0.5 (CN_fallow - CN_crop) = 0.5 CN_fallow + 0.5 CN_crop CN6 = CN_fallow
10	NCPDS	Number of cropping periods	Set to 26 (includes 6 warmup years for eventual buildup of residues)
11	EMD	Integer day of crop emergence	Set to same value as GDUSLEC1 for each cropping period

11	EMM	Integer month of crop emergence	Set to same value as GMUSLEC1 for each cropping period
11	IYREM	Integer year of crop emergence	Enter last two digits of each simulation year. The simulation period has to be adjusted such that there are no problems with the year 2000 (PRZM cannot handle it because the year has only two digits) or with leap years.
11	MAD	Integer day of crop maturation	Set to same value as GDUSLEC4 for each cropping period
11	MAM	Integer month of crop maturation	Set to same value as GMUSLEC4 for each cropping period
11	IYRMAT	Integer year of crop maturation	Enter last two digits of each simulation year. The simulation period has to be adjusted such that there are no problems with the year 2000 (PRZM cannot handle it because the year has only two digits) or with leap years.
11	HAD	Integer day of crop harvest	Set to same value as GDUSLEC5 for each cropping period
11	HAM	Integer month of crop harvest	Set to same value as GMUSLEC5 for each cropping period
11	IYRHAR	Integer year of crop harvest	Enter last two digits of each simulation year. The simulation period has to be adjusted such that there are no problems with the year 2000 (PRZM cannot handle it because the year has only two digits) or with leap years.
11	INCROP	Crop number	Set to 1 (there is only one crop)
12	PTITLE	Label for pesticide title	String composed of Koc reference, DT50 reference, crop reference and application month reference
13	NAPS	Total number of pesticide applications occurring at different dates	Set to 26 (one application per year).

13	NCHEM	Number of pesticides in the simulation	Set to 1.
13	FRMFLG	Flag for testing of ideal soil moisture conditions for the application of pesticides relative to the target date	Set to 0 (no testing) in accordance with FOCUSsw.
13	DKFLG2	Flag to allow input of biphasic degradation behaviour	Set to 0 (corresponds to FOCUS default).
15	PSTNAM	Name of pesticide for output titles	String composed of Koc reference, Koc value (in parentheses), DT50 reference and DT50 value (in parentheses)
16	APD	Integer target application day	Application date is determined based on the rainfall pattern in the application month with the following procedure: 1. Start with day 15 of the month 2. IF (Less than 20mm of rainfall the preceding day) AND (Less than 5mm of rainfall the 9 hours preceding application) THEN Application day 3. If conditions not satisifed, try day 14, then 16, then 13, then 17 and so on
16	AMD	Integer target application month	Set to the same value for each application year.
16	IAPYR	Integer target application year	Pesticides are applied once per simulation year.

16	WINDAY	Number of days in which to check soil moisture values following the target date for ideal pesticide applications	Set to zero (not used)
16	CAM	Chemical application method	Set to 2 (interception based on crop canopy, as a straight-line function of crop development; chemical reaching the soil is incorporated to 4 cm depth with concentration linearly decreasing with depth.
16	DEPI	Depth of the pesticide application (cm)	Set to 0 (not used if CAM = 2)
16	TAPP	Target application rate of the pesticide (kg ha^{-1})	Set to 1.
16	APPEFF	Application efficiency (fraction)	Set to 1 (in accordance with FOCUS).
16	DRFT	Spray drift (fraction).	Set to 0 (in accordance with FOCUSsw). In FOOTPRINT, drift is calculated outside PRZM.
17	FILTRA	Filtration parameter	Set to 0 (not used if CAM = 2)

17	IPSCND	Condition of foliar pesticide after harvest.	Set to 2 (2 = complete removal). Makes more sense than FOCUS setting (1 = surface applied).
17	UPTKF	Plant uptake factor	Set to 0.5 (FOCUSsw default for systemic pesticides). Yet, also non-systemic pesticides may be taken up by roots with the transpiration flux (they are just not translocated within the plant). The default value of 0.5 can therefore be used for all nonionic pesticides.
18	PLVKRT	Pesticide volatilization rate constant on plant foliage (d^{-1})	Set to 0 (in accordance with FOCUSsw).
18	PLDKRT	Pesticide decay rate constant on plant foliage (d^{-1})	Set to 0.06932 (corresponding to a foliar half-life of 10 days). This parameter is used in FOOTPRINT and FOCUS as a lumped dissipation rate constant (including also volatilization).
19	FEXTRC	Foliar extraction coefficient (cm^{-1}) for pesticide washoff per centimeter of rainfall	Set to 0.5 (FOCUSsw recommendation in absence of data on water solubility).
19	STITLE	Label for soil properties title	Set to the FOOTPRINT Unique Numbering. Uniquely identifies each of the FOOTPRINT model runs
20	CORED	Total depth of soil core (cm)	Set FST-specifically. Hard rock horizons are excluded from CORED.
20	BDFLAG	Bulk density flag	Set to 0 in accordance with FOCUSsw (bulk density directly entered in record 33).

20	THFLAG	Field capacity and wilting point flag	Set to 0 in accordance with FOCUSsw (water contents are directly entered in record 37).
20	KDFLAG	Soil adsorption flag	Set to 2 in accordance with FOCUSsw (normalized Freundlich equation).
20	HSWZT	Drainage flag	Set to 0 in accordance with FOCUSsw (free drainage). Restricted drainage would be interesting for some soils but this piece of code doesn't work.
20	MOC	Method of char-acteristics flag	Set to 0 in accordance with FOCUSsw (MOC not used).
20	IRFLAG	Irrigation flag	Set to 0 in accordance with FOCUSsw (irrigation not simulated). In FOOTPRINT and FOCUS, irrigation is included in the rainfall time series.
20	ITFLAG	Soil temperature simulation flag	Set to 2 (temperature- and moisture-dependent degradation rate). This option is used in FOCUSsw when laboratory degradation data are used.
20	IDFLAG	Thermal conductivity and heat capacity flag	Set to 1 in accordance with FOCUSsw (PRZM simulate temperature profile using default thermal conductivity and heat capacity, calculated from…).
20	BIOFLG	Biodegradation flag	Set to 0 in accordance with FOCUSsw (microbial population degradation algorithms not used).
26	DAIR	Diffusion coefficient for the pesticide in air (cm^2 d^{-1})	Set to 4300 in accordance with FOCUSsw.
26	HENRYK	Henry's Law constant of the pesticide (dimensionless)	Set to 0 (leads to zero volatilization). Since we simulate dummy substances, we can only make assumptions on Henry's Law constant. The assumption of no volatilization is a conservative one and therefore more appropriate in this case than the choice of a hypothetical HENRYK value > 0.

26	ENPY	Enthalpy of vaporization of the pesticide (kcal mol^{-1})	Set to 22.7 in accordance with FOCUSsw.
30A	FRNDCF	Freundlich exponent	Set to 1 (linear sorption). For the metamodelling, nonlinear sorption could not be considered, because then sorption would also depend on the application rate. → Additional to Koc and DT50, two more dimensions (Freundlich exponent and application rate) would have been necessary to create the metamodel database.
31	ALBEDO	Monthly values of soil surface albedo	Set to 0.18 for each month in accordance with FOCUSsw.
31	EMMISS	Emissivity of the soil surface for longwave radiation (fraction)	Set to 0.96 in accordance with FOCUS:
31	ZWIND	Height of wind speed measurement above the soil surface (m)	Set to 10 m, which corresponds to the weather stations whose data were used to generate the PRZM met files.
32	BBT	Average monthly values of soil temperatures (°C) at the bottom boundary of the profile	Set to annual average air temperature in accordance with FOCUS. FCZ BBT 1 12.1 2 10.5 3 9.1 4 4.9 5 12.4 6 9.1

			7 10.0 8 17.5 9 16.7 10 2.9 11 13.5 12 8.0 14 8.9 15 5.7 16 7.1
32A	QFAC	Q_{10} factor for degradation rate increase when temperature in-creases by 10 °C	Set to 2.2 in accordance with FOCUSsw (corresponding to an activation energy of 54 KJ mol^{-1})
32A	TBASE	Reference temperature for entered degradation rate constants	Set to 20 °C (most common value in degradation studies).
32B	ABSREL	Flag for type of reference soil moisture (absolute or relative to FC)	Set to 2 (= relative; i.e. values are entered in % of field capacity)
32B	B-VALUE	Exponent for moisture correction of degradation rate	Set to 0.7 (FOCUSsw default value).

32B	REFMOIST	Reference soil moisture for moisture correction of degradation rate	Set to 100 (= 100 % of field capacity)
33	NHORIZ	Total number of horizons	Specific for each FST. Horizons with upper boundary > 10 cm depth and lower boundary < 10 cm depth were split in two at 10 cm depth.
Note: Records 34-38 are to be entered in blocks for each horizon. First, the uppermost horizon is specified completely, then the next one, and so on.			
34	HORIZN	Horizon number	(running from 1 to NHORIZ)
34	THKNS	Thickness of the horizon	FST- and horizon-specific. Note that horizon boundary depths (and thus thickness) beyond 10 cm soil depth have been rounded to multiples of 5 cm. This was necessary because the numerical layers below 10 cm soil depth are 5 cm thick.
34	BD	Dry bulk density (g cm^{-3})	FST- and horizon-specific.
34	THETO	Initial volumetric soil water content in the horizon (cm^3 cm^{-3})	Set equal to field capacity (parameter THEFC) in accordance with FOCUSsw.
34	AD	Soil drainage parameter (d^{-1})	Set to 0 in accordance with FOCUSsw (option not used).
34	DISP	Pesticide hydro-dynamic dispers-ion coefficient (cm^2 d^{-1})	Set to 0 in accordance with FOCUSsw (dispersion is simulated numerically).

34	ADL	Lateral soil drainage parameter (d^{-1})	Set to 0 in accordance with FOCUSsw (option not used).
36	DWRATE	Dissolved phase pesticide degradation rate constant (d^{-1})	Specific for each dummy substance (ln2 / DT50). Correction of degradation rates with depth is done according to FOCUS: depth (cm) depth degradation rate correction factor 0-30 1 30-60 0.5 60-100 0.3 >100 0
36	DSRATE	Adsorbed phase pesticide degradation rate constant (d^{-1})	Same value as for DWRATE. Same correction with depth.
36	DGRATE	Vapour phase pesticide degradation rate constant (d^{-1})	Set to 0 in accordance with FOCUSsw.
37	DPN	Thickness of numerical compartments in the horizon (cm)	Set to 0.1 for 0-10 cm depth and to 5 for depths > 10 cm, in accordance with FOCUSsw.

37	THEFC	Field capacity water content in the horizon (cm^3 cm^{-3})	Based on pedotransfer functions for water content in the PRZM Manual corresponding to pF 2.5 (FC) and pF 4.2 (WP). The formulae used here additionally ensure that WP < FC and FC < PV, and they account for the presence of stones: FC = MIN [(0.3486 – 0.0018 SAND + 0.0039 CLAY + 0.0228 OM – 0.0738 BD) * (1-FSTONES); PV - 0.002] WP = MIN [(0.0854 – 0.0004 SAND + 0.0044 CLAY + 0.0122 OM – 0.0182 BD) * (1-FSTONES); FC - 0.01] *with* SAND = sand content (% of mineral component of fine earth) CLAY = clay content (% of mineral component of fine earth) OM = organic matter content (% of fine earth) BD = bulk density (kg/dm3); only refers to fine earth (< 2 mm) FSTONES = volumetric fraction of stones = Vstones/Vtot PV = pore volume fraction = Vpores / Vtot (dm3/dm3) PV in turn is calculated as: PV = [1 - (fOM * BD)/rhoOM - (1 - fOM) * BD/rhoMin] * (1 - FSTONES) fOM = gravimetric organic matter content, expressed as a fraction (kg/kg) rhoOM = substance density of organic matter (kg/dm3); assumed as 1.1 g cm^{-3} rhoMin = substance density of mineral soil components (kg/dm3), assumed as 2.65 g cm^{-3}
37	THEWP	Wilting point water content in the horizon (cm^3 cm^{-3})	
37	OC	Organic carbon content in the horizon (mass-%)	FST- and horizon-specific.
37	KD	Freundlich adsorption coefficient Kf (L kg^{-1})	FST-, horizon- and pesticide-specifc. Calculated as KD = K_{oc} * OC/100.
38	SPT	Initial temperature of the horizon (°C)	Set to BBT in accordance with FOCUSsw. This can be done because we have 6 warmup years.
38	SAND	Sand content (%)	FST- and horizon-specific.
38	CLAY	Clay content (%)	FST- and horizon-specific.

38	THCOND	Thermal conductivity of the horizon	Set to 0 in accordance with FOCUS (parameter not used if IDFLAG = 1)
38	VHTCAP	Heat capacity per unit volume of the soil horizon	Set to 0 in accordance with FOCUS (parameter not used if IDFLAG = 1)
40	ILP	Flag for initial pesticide concentrations in soil before start of simulation	Set to 0 in accordance with FOCUS (no initial pesticide concentration in soil profile).
Record 42 controls the .out output file, which is however not further used in FOOTPRINT. It’s only generated for control purposes.			
42	ITEM1	Hydrologic hardcopy output flag	Insert WATR (water variables are output)
42	STEP1	Time step of hydrologic output	Insert YEAR (yearly output)
42	LFREQ1	Frequency of hydrologic output given by a specific compartment number	Set to 5.
42	ITEM2	Pesticide flux output flag	Insert PEST (pesticide flux variables are output)

42	STEP2	Time step of pesticide flux output	Insert YEAR (yearly output)
42	LFREQ2	Frequency of pesticide flux output given by a specific compartment number	Set to 5.
42	ITEM3	Pesticide concen-tration output flag	Insert CONC (pesticide concentration variables are output)
42	STEP3	Time step of pesticide concen-tration output	Insert YEAR (yearly output)
42	LFREQ3	Frequency of pesticide concen-tration output given by a specific compartment number	Set to 5.
42	EXMFLG	Flag for reporting output to file for EXAMS model	Set to 0 (no output to EXAMS).
Records 45 and 46 control the .zts output file, whose content is used and further processed in FOOTPRINT. While record 45 specifies the number of output variables for which time series are to be plotted and the time step, record 46 contains plotting instructions and conversion factors for output to the zts file.			

45	NPLOTS	Number of time series plots (max = 12)	Set to 6 (6 output time series)
45	STEP4	Output time step	Set to DAY (daily output)
46	PLNAME	Name of plotting variable	PLNAME: The following output variables are chosen: 1. RUNF (surface runoff flux) 2. ESLS (eroded soil lost from field) 3. PRCP (precipitation) 4. TETD (total daily evapotranspiration) [only for control purposes] 5. RFLX1 (pesticide surface runoff flux) 6. EFLX1 (pesticide erosion flux)
46	INDX	Index to identify which pesticide if applicable	Set to 1 (there is only one pesticide).
46	MODE	Plotting mode: TSER, TCUM, TAVE, TSUM	Set to TSER (= daily time series) for all output variables
46	IARG	Argument value for PLNAME	Set to 0 (no arguments needed for the chosen output variables).
46	IARG2	Argument value for PLNAME	Set to 0 (no arguments needed for the chosen output variables).
46	CONST	Constant with which to multiply for conversion.	CONST: The same conversion factors and thus output units as in FOCUSsw are used. 1. RUNF: use conv. factor of 10 to convert cm to mm 2. ESLS: use conv. factor of 1000 to convert tonne to kg 3. PRCP: use conv. factor of 10 to convert cm to mm

			4. TETD: use conv. factor of 10 to convert cm to mm 5. RFLX1: use conv. factor of 10^7 to convert g cm^{-2} to mg m^{-2} 6. EFLX1: use conv. factor of 10^7 to convert g cm^{-2} to mg m^{-2}
			Record 46 finally looks this way: RUNF TSER 0 0 10.0 ESLS TSER 0 0 1.E3 PRCP TSER 0 0 10.0 TETD TSER 0 0 10.0 RFLX1 TSER 0 0 1.E7 EFLX1 TSER 0 0 1.E7

3 AUTOMATION OF MODELLING ACTIVITIES

The FOOTPRINT work involves the running of the two pesticide fate models PRZM and MACRO for several millions of time and PRZM modelling tasks were therefore fully automated. These comprised the preparation and formatting of PRZM input files, the running of the model, the extraction of statistics of interest and the archiving of model output files. Full automation was achieved through a combination of macros written in Visual Basic and scripts written in Perl. A total of 3 automation modes were developed: 1) One-at-a-time; 2) Generation of input files; and, iii) Batch mode.

In the *one-at-a-time mode*, MS Excel is used to create two text files (master.txt and master2.txt) containing a unordered list of all PRZM input parameters and the associated values for a given combination of climate, soil, crop, application date, Koc and DT50. A perl script is then used to read the parameter values listed in the two text files and prepare the .inp and .run input files according to the PRZM formatting requirements. The one-at-a-time also allows the PRZM output files to be post-processed automatically to derive meaningful statistics. The one-at-a-time mode which is controlled through an interface in MS Excel is designed to allow the preparation of PRZM input files, to run the model and to extract model output information for one run only. It is used by FOOTPRINT modellers to evaluate the fate of specific pesticides in specific scenarios and to check results coming out of complex perl scripts.

In the *Generation of input files mode*, the user is invited to list the combinations of climate, soil and crop he is interested in. A loop goes through the various combinations listed and uses the one-at-a-time automation routines described above (combinations of VB and perl scripts) to generate series of 1404 input files for each combination of climate, soil and crop. The 1404 input files cover all combinations of Koc, DT50 and application dates listed in the FOOTPRINT database. The 1404 files are finally compressed together in a rar file which takes the name of the climate, soil and crop combination. The generation of input files mode is used by FOOTPRINT modellers to prepare a large number of input files to be run on the FOOTPRINT@work distributed system.

In the *batch* mode, the user is invited to list the combinations of climate, soil, crop, application date, Koc and DT50 he is interested in. A loop will go through the combinations listed, generate all relevant input files, run PRZM repeatedly and then postprocess results for all the output files created by the model. The batch mode is use by FOOTPRINT modellers to undertake a limited number of automated runs.

4 CONCLUSIONS AND PERSPECTIVES

The present report has described a logically consistent and complete parameter database for the pesticide fate model PRZM. The corresponding MS Excel macros and perl scrips allow the preparation of model input files based on widely available data, the running of the model and the postprocessing of model outputs. The database contains PRZM parameters for 16 FOOTPRINT climate zones (FCZ), 264 agriculturally-relevant FOOTPRINT soil types (FST) and 42 FOOTPRINT crops (FCR), allowing simulations of pesticide losses from fields via surface runoff and erosion for all agriculturally relevant agro-environmental scenarios in the EU25.

5 REFERENCES

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