Version: 2.0
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PRZM - Parameterisation for the FOCUS Groundwater Scenarios

About this document

The reports on which this document is based are those of the FOCUS Groundwater Scenarios workgroup (FOCUS, 2000) and the FOCUS Ground Water Work Group (FOCUS, 2009). This document does not replace the official FOCUS reports. 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

Together with the "FOCUS PRZM GROUNDWATER TOOL VERSION 2.2.1 (FEBRUARY 2001)" a new version of the PRZM simulation model (VERSION 3.21 BETA, FOCUS RELEASE, FEBRUARY 2001) has been issued. Necessary changes to keep the parameterisation document up-to-date with the model are incorporated in this new version controlled document. The only other changes in this version compared with the original report are editorial ones.

New in Version 2.0

This version incorporated the changes resulting from the implementations of the recommendations from the FOCUS Ground Water Group report (FOCUS 2010). This report describes FOCUS PRZM Ground Water Tool Version 3.5.2, using WINPRZM 4.5.1

1 Summary

PRZM is a one dimensional finite-difference model for prediction of the vertical movement of chemicals in soil by chromatographic leaching. The first official version (Carsel *et al*., 1984) was released in 1984 although beta versions were available from 1982. An upgraded version PRZM2 was issued as part of the RUSTIC package (Dean *et al*., 1989a & 1989b) and later as a stand-alone model. In the mid-1990's the runoff routines were upgraded as part of the work of the FIFRA Exposure Modelling Work Group and the FIFRA Environmental Model Validation Task Force to produce version 3.12. This version also included more flexibility with application techniques, the ability to make degradation a function of soil temperature, and output which is more user friendly. Version 3.12 is also the version that has been used by the FIFRA Environmental Model Validation Task Force in its program to compare model predictions with actual data from runoff and leaching field studies. For use in the FOCUS scenarios, version 3.21 was developed, which in addition to the capabilities of version 3.12 has the option of using the Freundlich isotherm, the ability to make the degradation rate a function of soil moisture, the capability to consider increasing sorption with time and implementation of exact first order kinetics for metabolites. The version used to implement the recommendations of FOCUS (2010) is WINPRZM 4.51.

Table 1.1 Summary of the processes in WINPRZM 4.51 (FOCUS release, December 2010)

Process	Approach
water movement	capacity-based water flow (tipping bucket approach) using a daily time step for all hydrological processes, option for Richard's equation below the root zone. *Preferential flow, capillary rise and drainage not considered
substance movement	convection dispersion equation based on a daily time step solved by an simplifying backward difference method which can produce artificially high numerical dispersion
crop simulation	changing root zone during growing season, changing foliage (both height and areal extent) during growing season, crop interception of water*, crop interception of substances*, foliar washoff*, foliar degradation*
degradation in soil	first order degradation rate with option for bi-phasic degradation, option for effects of soil temperature and moisture on degradation
substance sorption to soil	Kd, Koc, or normalised Freundlich equation for sorption; option for increasing sorption with time.
substance volatilisation (from soil)	approach is a combination of results from previous research
runoff	Soil Conservation Service curve number technique (not used in Tier 1)
soil erosion*	Universal Soil Loss Equation
soil temperature	Approach is based on previous work by a number of researchers inc. Van Bavel and Hillel, Thibodeaux, Hanks, Gupta, and Wagenet and Hutson
plant uptake	simple model based on soil concentrations
substance applications	applications may be foliar sprays*, applied to the soil surface, or incorporated into the soil; for soil incorporated applications a variety of soil distributions can be specified
metabolism	up to two metabolites may be simulated simultaneously with the parent

*process not used in FOCUS scenarios

Development of Parameter Sets

The development of input parameter sets from the weather, soil, and crop information was generally straightforward. Details are provided in the appendix providing values of all of the input parameters. Dispersion length was determined to correspond to a value 5 cm as prescribed by FOCUS (2009). Crop specific runoff curve numbers were determined from the information in the PRZM 3.12 manual assuming a SCS hydraulic soil group of A for Piacenza, B for Hamburg and C for the rest of the locations. However, this is turned off for Tier 1 simulations

2 Introduction

A modified and improved PRZM code (version 4.51, FOCUS release) is used with the FOCUS shell.

The PESTICIDE ROOT ZONE MODEL executable PRZM31.EXE as well as all former PRZM versions run under Microsoft DOS. In order to realise a truly Windows based PRZM the program code was re-coded and compiled with a 32 bit FORTRAN compiler. The new PRZM4.51 executable WINPRZM.EXE is independent from any DOS limitations and can be run with either or 32 or 64 bit operating system. A windows shell called FGRAT.EXE (FOCUS Groundwater Risk Assessment Tool) was built around the new PRZM executable to make the creation of PRZM input files easier. The shell is optimised for a screen resolution of 1024x768 pixel and provides the following features:

- user-friendly scenario and parameter definitions a Microsoft Windows environment.
- pre-definition of the European FOCUS Tier 1 groundwater scenarios.
- modified and enhanced PRZM4.51 code.

The information necessary to run PRZM4.51.EXE is divided into a number of input data files:

- climate file providing the weather data *.met
- parameter file including the scenario definition *.inp
- file with definition of the PRZM run options *.run

The shell FGRAT.EXE facilitates the creation of the required input files by the user. In addition a file of the type *.scn is created to support the grapher of the PRZM shell with necessary information for the data analysis.

All scenario and compound specific information necessary to characterise the whole simulation project in the selected working directory is summarised by the FOCUS PRZM Shell in one Master Project file called “master.fpj”. This Master Project file is the only file needed by the PRZM shell to re-generated the full simulation scenario including all necessary PRZM input files. Thus the Master Project may be used for an easy exchange of simulation scenarios.

The implemented scenario and parameter definitions are based on:
FOCUS DEFINITION = Definitions made by the FOCUS working group
DEVELOPMENT DEFINITION = Definitions made during the PRZM FOCUS shell development
USER INPUT = Input to be specified by the user in the PRZM FOCUS shell

Parameter definitions based on **FOCUS** or **DEVELOPMENT DEFINITION** are not changeable by the user in the PRZM FOCUS shell. Several parameter can be specified based on the **USER INPUT**, but only according to a selection of predefined values based on **FOCUS** or **DEVELOPMENT DEFINITION**. In such cases the parameter definition is called **FOCUS SCENARIO SPECIFIC**. Other parameters may be defined in the shell without such limitations. Nevertheless, it is possible to change all predefined and generated data files manually, outside the PRZM FOCUS shell. For FOCUS Tier 1 simulations none of the shell-generated data files should be modified.

After a completed simulation run, the relevant scenario output data is given in six ASCII files of the type *.ann, *.hyd, *.cnc, *.msb, *.out and *.zts. The shell will analyse those files

automatically and provide the user with result tables and graphics, with the information specified by FOCUS.

3 Parameter description

PARAMETER AND DESCRIPTION		VALUE, SOURCE & COMMENTS
Meteorological files		
MMDDYY:	meteorological month/day/year	Used are 9 location specific weather scenarios and 24 crop and location specific irrigated weather scenarios. All 66 year FOCUS weather files are given in the NOAA-format (NOAA = National Oceanographic and Atmospheric Administration). - **FOCUS SCENARIO SPECIFIC**
PRECIP:	precipitation (cm day^{-1})	
PEVP:	pan evaporation data (cm day^{-1})	
TEMP:	temperature (Celsius)	
WIND:	wind speed (cm sec^{-1})	
SOLRAD:	solar radiation (Langley)	
Record 1		
TITLE:	label for simulation title	**FOCUS SCENARIO SPECIFIC**
Record 2		
HTITLE:	label for hydrology information title	**FOCUS SCENARIO SPECIFIC**
Record 3		
PFAC:	pan factor used to estimate the daily potential evapotranspiration (ET) from the daily pan evaporation.	**FOCUS DEFINITION** - crop specific values are defined by the crop specific kc factors, (see record 9A).
SFAC:	snowmelt factor in cm/degrees Celsius above freezing.	set to **0.46** - **DEVELOPMENT DEFINITION** - SFAC is an empirical factor with wide variation. The value 0.46 represents an appropriate average based on data in the PRZM 3.12 manual and on Anderson, E.A.; 0.46 is also default value in PELMO 2.0
IPEIND:	pan factor flag	set to 7 = daily pan evaporation is read from the meteorological file - ET modified by crop growth stage **FOCUS DEFINITION**
ANETD:	minimum depth of which evaporation is extracted (cm).	**DEVELOPMENT DEFINITION** - The following values are suggested for the specific FOCUS scenarios (see Focus, 2009 for the explanation of the values for Piacenza, Sevilla, and Thiva): CHÂTEAUDUN C **20 cm** HAMBURG H **15 cm** JOKIOINEN J **10 cm** KREMSMÜNSTER K **15 cm** OKEHAMPTON N **15 cm** PIACENZA P **15 cm** PORTO O **25 cm** SEVILLA S **15 cm** THIVA T **20 cm** Comment: This value represents soil evaporation moisture loss during a fallow, dormant period. By default evaporation is assumed to occur in the top 10 cm of soil with remaining moisture losses occurring below 10 cm up to the maximum rooting depth. Values for ANETD apply only when there is no growing season, allowing a reduced level of moisture loss through evaporation limited to the minimum depth.
INICRP:	flag set to use an initial crop before first emergence.	set to 1 = simulate initial crop - **DEVELOPMENT DEFINITION** set to 1 = fallow - **DEVELOPMENT DEFINITION**
ISCOND:	surface condition of initial crop	not used in the input files - **DEVELOPMENT DEFINITION**

DSN:	WDM data set (5 numbers)	
Record 6		
ERFLAG:	flag to select simulation of erosion.	set to 0 = **no** erosion - **FOCUS DEFINITION**
Record 8		
NDC:	number of different crops in the simulation.	set to 1 = only **one** crop - **FOCUS DEFINITION**
Record 9		
ICNCN:	crop number of the different crop.	set to 1 = the one crop used - **FOCUS DEFINITION**
CINTCP:	maximum interception storage of the crop (cm).	set to zero = no rainfall interception - **FOCUS DEFINITION**
AMXDR:	maximum rooting depth of the crop (cm).	**FOCUS SCENARIO SPECIFIC**
COVMAX:	maximum areal coverage of the canopy (percent).	**FOCUS SCENARIO SPECIFIC** - is set to the maximum interception percentages (crop and location specific values vary from 45% to 90%)
ICNAH:	surface condition of the crop after harvest date (fallow, cropping, residue).	set to 3 = residue - **DEVELOPMENT DEFINITION**
CN:	runoff curve numbers of antecedent moisture condition II for fallow, cropping, residue (3 values).	Runoff is calculated by a modification of the USDA Soil Conservation Service curve number approach (Haith *et al*., 1979). The curve numbers were selected based on two definitions: Curve numbers of 0 are to be used for Tier 1 scenarios. The following are the numbers that are used when runoff is simulated. 1) **SCS hydraulic Soil Group:** The SCS group was chosen for Piacenza to be **A**, Hamburg to be **B** and for all the rest locations to be **C** - **FOCUS DEFINITION** 2) **Curve Numbers:** Crop and soil specific CN are defined corresponding to values of PELMO 2.0, the original USDA definition and the PRZM 3.12 manual. - **DEVELOPMENT DEFINITION**

SCS soil group:	**A**	**B**	**C**	**D**	HTMAX	PFAC
– fallow + residue	77	86	91	94	-	1.00
– apples (orchards)	36	60	73	79	250	0.99
– grass(+alfalfa)	30	58	71	78	40	1.00
– potatoes	62	83	89	93	100	0.94
– sugar beet	58	72	81	85	40	0.93
– winter cereals	54	70	80	85	100	0.84
– beans (field+vegetable)	67	78	85	89	150	0.89
– bush berries	36	60	73	79	130	1.00
– cabbage	58	72	81	85	30	0.97
– carrots	58	72	81	85	40	0.96
– citrus	36	60	73	79	250	0.73
– cotton	67	78	85	89	120	0.95
– linseed	54	70	80	85	150	0.84
– maize	62	83	89	93	250	0.94
– oil seed rape (sum)	54	70	80	85	140	0.93
– oil seed rape (win)	54	70	80	85	140	0.78
– onions	58	72	81	85	60	0.91
– peas (animals)	67	78	85	89	100	0.96
– soybean	67	78	85	89	170	0.92
– spring cereals	54	70	80	85	110	0.92
– strawberries	58	72	81	85	40	1.00
– sunflower	62	83	89	93	150	0.86
– tobacco	67	78	85	89	250	0.98
– tomatoes	62	74	81	86	110	0.97

– vines 45 62 73 79 170 0.89	
	For all perennial crops (alfalfa, apples, bush berries, citrus, grass, strawberries, vines) the same CN are used for fallow and residue!
WFMAX: maximum dry weight of the crop at full canopy (kg m^{-2}).	set to 0.0 = not used - **FOCUS DEFINITION** (only required if non-linear foliar application).
HTMAX: max. canopy height at maturation date (cm).	**DEVELOPMENT DEFINITION** - crop specific rough estimates are given in foregoing table with CN Comment: HTMAX is used in PRZM to calculate the substance volatilisation. Canopy height increases during crop growth resulting in substance flux changes in the plant compartment. The suggested HTMAX estimates are only crop and not site specific.
Record 9A KCINIT: **Harvest to Emergence** KCMID: **Emergence to Maximum LAI** KCLATE: **Senescence to Harvest** KCMAX: **Maximum LAI to Senescence**	**Kc factor as a function of Cropping Periods (expressed in dd/mm-dd/mm) - FOCUS SCENARIO SPECIFIC**
Record 10 NCPDS: number of cropping periods.	set to 26, 46 or 66 - **FOCUS SCENARIO SPECIFIC**
Record 11 (repeated up to NCPDS) E_DDMMYY: crop emergence date (month/day/year). M_DDMMYY: crop maturation date. H_DDMMYY: crop harvest date. INCROP: crop number associated with NDC P10_DDMMYY: Date of Maximum LAI P60_DDMMYY: Date of Senescence	**FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC** set to 1 (only one crop) - **FOCUS DEFINITION**
Record 13 NAPS: total number of substance applications occurring at different dates (1 to 50). NCHEM: number of substance(s) in the simulation. FRMFLG: flag for testing of ideal soil moisture conditions for the application of substance relative to the target date. DKFLG2 flag to allow input of bi-phase half-life.	**FOCUS SCENARIO SPECIFIC / USER INPUT** (User can specify in the PRZM shell up to 10 annual substance applications.) **USER INPUT** set to 1 = parent only set to 2 = parent with metabolite set to 3 = parent with two metabolites set to 0 = **no** moisture test - **FOCUS DEFINITION** **USER INPUT** default = set to 0 = **no** bi-phase half-life Comment: The PRZM FOCUS shell offers the option to activate a bi-phase half-life if experimental data is available.

Record 14 **(only if DKFLG2 = 1)**		
DKDAY:	day when first half-live begins	**USER INPUT**
DKMNTH:	month when first half-live begins	**USER INPUT**
DKNUM:	number of days after begin of first half-live to swap from first to second bi-phase half-live	**USER INPUT**
Record 15		
PSTNAM:	name of substance(s) for output file.	**USER INPUT**
Record 16		
AP_DDMMYY:	target application date.	**USER INPUT** default = one day before emergence
WINDAY:	number of days in which to check soil moisture values following the target date for ideal substance(s) applications.	set to 0 = not used - **FOCUS DEFINITION** (only required if FRMFLG = 1)
CAM:	flag set to select application method.	**USER INPUT** Selectable chemical application methods are: **1** = soil applied, default incorporation depth = 4 cm, linearly decreasing with depth. This is the **DEFAULT** to be used for FOCUS TIER 1 modelling. **2 =** linear foliar based on crop canopy, default soil incorporation depth for non-foliar intercepted chemical is 4 cm, linearly decreasing with depth; **3** = non-linear foliar using exponential filtration, same default soil incorporation as in CAM = 2; **4** = soil applied, user defined incorporation depth (DEPI), uniform with depth; **5** = soil applied, user defined incorporation depth, linearly increasing with depth; **6** = soil applied, user defined incorporation depth, linearly decreasing with depth; **7** = soil applied, T-Band granular application, user defined incorporation depth; **8** = soil applied, chemical incorporated entirely into depth specified by user. **Note:** Foliar application needs to be activated in PRZM to simulate washoff from plant foliage and degradation of foliage substance. Degradation of compound in plants after plant uptake is not simulated in PRZM!
DEPI:	incorporation depth of substance application (cm). DEPI must be used with CAM = 4, 5, 6, 7 and 8. Default value for CAM = 2 or 3 may be over-ridden by entering another value. DEPI must be always set greater than 0 (PRZM requirement)!	**USER INPUT** **Note:** To **prevent an overprediction of runoff** the default PRZM DEPI of 4 cm (linearly decreasing with depth) must be used for applications made to the soil surface. Actual runoff results and experience suggest that this PRZM default is much more appropriate to simulate 'realistic' runoff than a thin-layer soil surface application!
$TAPP_i$:	target application rate (kg ha^{-1}).	**USER INPUT**
$APPEFF_i$:	application efficiency (fraction).	**USER INPUT** default = set to 1 (no application loss) Default value not to be changed for TIER 1 modelling!
$DRFT_i$:	spray drift (fraction).	

		USER INPUT default = set to 0 (no spray drift) Default value not to be changed for TIER 1 modelling! Comment: Index i is used to differentiate between parent and metabolites.
Record 17		
FILTRA:	filtration parameter. Only required if CAM = 3.	set to zero (as not required) - **FOCUS DEFINITION**
IPSCND:	condition for disposition of foliar substance after harvest (1 = surface applied, 2 = complete removal, 3 = left alone)	set to 2 - **FOCUS DEFINITION** (only required and used if foliar application, CAM = 2 or 3)
UPTKF:	plant uptake factor (between 0.000 and 1.0; describes uptake as a fraction of transpiration* dissolved phase concentration)	**USER INPUT** set to 0.5 for systemic compounds (default) set to 0 = **no** plant uptake for other compounds Other values not to be used for TIER 1 modelling!
Record 18	**(only if CAM = 2 or 3)**	
PLVKRT:	substance volatilisation decay rate on plant foliage ($days^{-1}$).	**USER INPUT** Not relevant for TIER 1 modelling since crop interception to be set to zero.
PLDKRT:	substance decay rate on plant foliage ($days^{-1}$).	**USER INPUT** Not relevant for TIER 1 modelling since crop interception to be set to zero.
FEXTRC:	foliar extraction coefficient for substance washoff per centimetre of rainfall	**USER INPUT** Not relevant for TIER 1 modelling since crop interception to be set to zero.
Record 19		
STITLE:	label for soil properties title.	**FOCUS SCENARIO SPECIFIC**
Record 20		
CORED:	total depth of soil core in cm.	**FOCUS SCENARIO SPECIFIC**
BDFLAG:	bulk density flag.	set to 0 = soil specific bulk density is used **- DEVELOPMENT DEFINITION**
THFLAG:	field capacity and wilting point flag.	set to 0 = the **FOCUS SCENARIO SPECIFIC** soil water contents are used - **DEVELOPMENT DEFINITION** Comment: another PRZM option would be to calculate field capacity and wilting point by using scenario specific clay and sand contents.
KDFLAG:	flag to select soil/substance adsorption coefficient (KD, Koc or normalised Freundlich using C_{ref} = 1 mg L^{-}, aged sorption KD_{aged}).	**FOCUS SCENARIO SPECIFIC** - set to 0, 2 or 3 depending on **USER INPUT**: **0** = KD values are calculated from the FOCUS PRZM shell for each layer (using Koc and OC) and entered in **Record 37**; **1** = layer specific KD are calculated from PRZM itself during the simulation using the Koc value entered in **Record 30** and layer specific OC; values in Record 37 are not used! **2** = normalised Freundlich equation is used; layer specific KD are calculated from the PRZM shell and entered in **Record 37**; Freundlich exponent 1/n is entered in **Record 30b**. **3** = Aged sorption is implemented: Compound specific ageing factors are defined in **Record 30c** and applied to

	calculated an aged sorption on a daily basis. Normalised Freundlich equation is used in the same way as described for **2**.
HSWZT: drainage flag.	set to 0 = free draining - **FOCUS DEFINITION**
MOC: method of characteristics flag. / kinetic sorption	set to 2 for Kinetic Sorption, set to 1 for MOC, set to 0 = not used - **DEVELOPMENT DEFINITION** Comment: flag is now dual purposed to turn on kinetic aged sorption when set = 2 Comment: The MOC algorithm is a two-pass solution technique first introduced with PRZM 3 in order to reduce truncation error and numerical dispersion for advection-dominated systems. Without using MOC artificial effects of numerical dispersion may appear in systems having high Peclet numbers (low Koc, high flow rate, sandy soils). Under vulnerable conditions it may be recommended to use MOC instead of the default backwards-difference solution algorithm, especially as there is in PRZM no automatic warning for an excessive numerical dispersion. **Without using MOC the numerical dispersion is for each scenario unknown, not predictable and has to be analysed manually using tracer data.** If the MOC algorithm is chosen, then a typical experimental value for field-observed data dispersion should be entered. Because of the 24 hour time step in PRZM, the MOC method can lead to significant losses of mass under high velocity (greater than 120 cm per day) conditions.
IRFLAG: irrigation flag.	set to 0 = no irrigation is simulated (necessary irrigation will be added in rainfall data) - **FOCUS DEFINITION**
ITFLAG: soil temperature simulation flag. (0 = off; 1 or 2 = on)	**FOCUS SCENARIO SPECIFIC** Comment: ITFLAG = 2 activates in this modified PRZM version the simulation of soil temperature **and** the use of temperature and moisture corrected degradation (laboratory degradation data)!
IDFLAG: flag to select thermal conductivity and heat capacity	set to 1 = PRZM simulates automatically soil temperature profiles without the need of thermal conductivity and heat capacity - **DEVELOPMENT DEFINITION** Comment: Thermal conductivity and heat capacity data is not specified in the FOCUS data.
BIOFLAG: biodegradation flag	set to 0 = special multiphase biodegradation using a detailed definition of micro-organism populations is **not** used - **FOCUS DEFINITION**
CNFLAG: curve number flag	set to 0 = no alternative methods for curve number calculations - **FOCUS DEFINITION**
DSPFLG: dispersion length flag	set to 1 = enter horizon specific dispersion length - **FOCUS DEFINITION**
Record 26 DAIR: molecular diffusion coefficient for the substance(s) in the air. (**cm^2 day^{-1}**)	set to 4300 = **FOCUS DEFINITION** (0.43 m^2day^{-1} = 4300 cm^2day^{-1})

HENRYK:	normalised Henry's law constant of the substance(s). (dimensionless)	set to a value calculated from the PRZM shell depending on other **USER INPUT** Comment: Henry's constant **H** is a ratio of a chemical's vapour pressure to its solubility. It represents the equilibrium between the vapour and solution phases. It is quite common to normalise **H** with R*T using T=20°C and to express **H** in this way as a dimensionless number (HENRYK): HENRYK = H / (R*T) = P*M / (C*R*T) P = vapour pressure (Pa) - **USER INPUT** M = mol weight (g $mole^{-1}$) - **USER INPUT** C = water solubility (mg L^{-1}) - **USER INPUT** R = gas constant = 8.3144 J K^{-1} $mole^{-1}$ T = absolute temperature (K)
$ENPY_i$:	enthalpy of vaporisation of the substance(s). (kcal $mole^{-1}$)	set to 22.7 kcal $mole^{-1}$ - **FOCUS DEFINITION** Comment: Index i is used for parent and metabolites.
Record 30 **(only if KDFLAG = 1)**		
PCMC:	flag to select which model is used to estimate KD (see record 37).	set to 4 = Koc in L kg^{-1} depending on **USER INPUT**
SOL:	substance(s) Koc entered according to PCMC flag above for each NCHEM.	**USER INPUT**
Record 30b **(only if KDFLAG = 2 or 3)**		
$FRNDCF_i$:	Freundlich exponent 1/n (dimensionless) The normalising reference concentration C_{ref} is fixed in the PRZM code to 1 mg L^{-1}. The use of the non-linear Freundlich is limited to a concentration higher than 1 x 10^{-20} µg L^{-1}.	**USER INPUT** Normalised Freundlich is implemented in PRZM in the same way as in PELMO and in PEARL. - **DEVELOPMENT DEFINITION** Comment: Value of Cref is necessary but not included in the definition of the FOCUS dummy substances! For the calculations a Cref of 1 mg L^{-1} was assumed. Index i is used to differentiate between parent and metabolites.
Record 30c **(only if KDFLAG = 3)**		
BAKD:	Time points for the definition of the ageing factors VAKD (days) - 5 values	**USER INPUT** Non-kinetic aged sorption is not normally used. Instead the kinetic sorption routines would normally be used..
VADK:	Time dependent factor (5 dimensionless values) to calculate an aged sorption: KD_{aged} = VADK * KD	Comment: Non-kinetic aged sorption is described with an dimensionless time dependent ageing factor VADK > 1. An ageing effect is often relevant for the behaviour of substances in soil and may be extracted from standard Ad-/Desorption studies as specified from the OECD (1997). The ageing factor is calculated on an daily basis by linear interpolation of the specified data and limited to the last of the five VADK numbers. After each application the ageing period is reset back to zero. This is done to prevent an over prediction of ageing.
Record 31 **(only if ITFLAG = 1 or 2)**		
ALBEDO:	monthly values of soil surface albedo - 12 values.	**DEVELOPMENT DEFINITION** - To simulate soil temperatures, the ALBEDO values were used in the PRZM runs. Since the albedo of soil surface changes with the soil surface condition, it is defined by the user as 12 monthly values corresponding to the first day of each month; the albedo value for each day is interpolated between the neighbouring monthly values. The soil ALBEDO factors were set to **0.18** (average for bare field and different bare soils under natural conditions). The

		albedo of a canopy-covered land surface is estimated by the model using the canopy cover. For snow cover less than 0.5 cm, the surface albedo is estimated, and for snow cover above 0.5 cm, the surface ALBEDO is set in PRZM automatically equal to **0.80** (fresh snow value). For January in Hamburg, January and February in Kremsmünster, and December, January, and February in Jokioinen the bare soil ALBEDO factors are set to **0.60** (old snow). (data based on the PRZM 3.12 manual).
EMMISS:	reflectivity of soil surface to longwave radiation (fraction).	**DEVELOPMENT DEFINITION** - Depending on soil moisture and crop this reflectivity varies in a narrow band between 0.94 and 0.98 for natural surfaces at normal temperatures. The average of **0.96** was used in the PRZM runs. (data based on PRZM 3.12 manual)
ZWIND:	height of wind speed measurement above the soil surface (m)	set to 10 m - **FOCUS DEFINITION**
Record 32 **(only if ITFLAG = 1 or 2)**		
BBT:	average monthly values of bottom boundary soil temperatures in degrees Celsius (12 values).	Location specific monthly bottom temperatures are calculated based on the FOCUS weather files as 20 year average air temperature for each location (values see under ANETD in Record 3) - **FOCUS DEFINITION**
Record 32a **(only if ITFLAG = 2)**		
$QFAC_i$:	Q10-factor for degradation rate increase when temperature increases by 10°C	**USER INPUT** default = 2.58 - **FOCUS DEFINITION**
$TBASE_i$:	temperature during the test of biodegradation	**USER INPUT** Comment: Index i is used for parent and metabolites.
Record 32b **(only if ITFLAG = 2)**		
$absrel_i$:	flag to select if reference soil moisture for moisture corrected degradation is given absolute or relative to FC (field capacity)	**USER INPUT** (absolut: absrel = 1; relative to FC: absrel = 2)
B-$value_i$:	exponent of moisture corrected degradation (moisture relationship according to WALKER)	**USER INPUT** default = 0.7 - **FOCUS DEFINITION**
$refmoist_i$:	reference soil moisture	**USER INPUT** Comment: Index i is used for parent and metabolites.
Record 33		
NHORIZ:	total number of horizons	**FOCUS SCENARIO SPECIFIC**
Record 34 **(repeat Records 34-38 up to NHORIZ)**		
HORIZN:	horizon number in relation to NHORIZ.	**FOCUS SCENARIO SPECIFIC**
THKNS:	thickness of the horizon.	
BD:	bulk density (kg/L).	**FOCUS SCENARIO SPECIFIC**
THETO:	initial soil water content in the horizon (cm^3 cm^{-3}).	**FOCUS SCENARIO SPECIFIC**
AD:	soil drainage parameter (day^{-1}). (only required if HSWZT = 1)	set to field capacity from FOCUS soil data - **DEVELOPMENT DEFINITION** set to 0 = not used - **FOCUS DEFINITION**
DISP:	substance(s) hydrodynamic solute dispersion/diffusion coefficient.	

(cm^2 day^{-1})	set to 0 - **DEVELOPMENT DEFINITION** (DISP is only used for MACRO and PEARL)
ADL: lateral soil drainage parameter (day^{-2}). (only required if HSWZT = 1).	set to 0 = not used - **FOCUS DEFINITION**
DISLEN: dispersion length for horizon (cm)	set to 5.0 - **DEVELOPMENT DEFINITION**
Record 36 **(for DKFLG2 = 0)**	
$DWRAT_i$: dissolved phase substance(s) decay rate for first phase (day^{-1}).	Based on a lumped degradation the two parameters $DWRAT_i$ and $DSRAT_i$ are set from the shell for each compound to the substance degradation rate specified by the **USER INPUT. - DEVELOPMENT DEFINITION**
$DSRAT_i$: adsorbed phase substance(s) decay rate for first phase (day^{-1}).	Comment: Index i is used for parent and metabolites.
$DGRAT_i$: vapour phase substance(s) decay rate for first phase (day^{-1}).	set to 0 - **DEVELOPMENT DEFINITION**
	Note: In this modified PRZM 3.20 the use of a metabolite transformation fraction was introduced as suggested by FOCUS (see also Record 39). Therefore each DWRAT represents now the total degradation rate of each compound (parent or metabolite). In addition the implementation of the first order degradation routines has been modified for from an approximation to an exact implementation of first order kinetics.
Record 36a **(only if DKFLG2 = 1)**	
$DWRAT2_i$: dissolved phase pesticide(s) decay rate for second phase of bi-phase reaction (day^{-1}).	Based on a lumped degradation the two parameters DWRAT2i and DSRAT2i are set from the shell for each compound (index I for parent and metabolites) to the same pesticide degradation rate specified by the **USER INPUT**. - **DEVELOPMENT DEFINITION**
$DSRAT2_i$: adsorbed phase pesticide(s) decay rate for second phase of bi-phase reaction (day^{-1}).	Comment: Index i is used for parent and metabolites.
$DGRAT2_i$: vapour phase pesticide(s) decay rate for second phase of bi-phase reaction (day^{-1}).	set to 0 - **DEVELOPMENT DEFINITION**
Record 37	
DPN: thickness of compartments in the horizon (cm).	0 - 10 cm: 0.1 cm thickness > 10 cm: 5.0 cm thickness - **FOCUS DEFINITION** for PRZM runs
	Comment: In general, a smaller DPN will generate more accurate results and provide greater spatial resolution, but will also consume more CPU time. From a volatilisation viewpoint, a smaller DPN in the top horizon is required for better estimation of the volatilisation flux from the soil surface. In addition, since substance runoff is calculated from the surface layer, a smaller layer depth allows a better representation of surface-applied chemicals. Values of 0.1 cm are recommended for the initial 10 cm of the soil profile and where volatilisation is a major loss mechanism (PRZM default, see PRZM 3.12 manual).
THEFC: field capacity in the horizon (cm^3 cm^{-3}).	**FOCUS SCENARIO SPECIFIC**
THEWP: wilting point in the horizon (cm^3 cm^{-3}).	**FOCUS SCENARIO SPECIFIC**
OC: organic carbon in the horizon (percent).	

KD:	layer specific substance(s) partition coefficient for each NCHEM. (L kg^{-1}).	**FOCUS SCENARIO SPECIFIC**
FEQ:	fraction of chemical subject to equilibrium sorption	**FOCUS SCENARIO SPECIFIC / USER INPUT** (required if KDFLAG = 0 or 2, else set to 0.0)
KDES:	desorption rate for non-equillibrium sorbed chemical	**USER INPUT –** Input as PEARL Factor in Shell, converted to FEQ for use in PRZM
DKS2:	degradation rate for non-equillibrium sorbed chemical (ln2/days)	**USER INPUT** set to 0 - **DEVELOPMENT DEFINITION** Comment: If more than 1 chemical, FEQ, KDES, and DKS2 for chemical 2 and 3 are placed on next line
Record 38	**(only if ITFLAG = 1 or 2)**	
SPT:	initial temp. of the horizon (Celsius).	calculated bottom temperatures - **DEVELOPMENT DEFINITION**
SAND:	sand content in the horizon (percent).	SAND and CLAY contents are set to 0 - values only required if THFLAG = 1
CLAY:	clay content in the horizon (percent).	- **DEVELOPMENT DEFINITION**
THCOND:	thermal conductivity of the horizon (cm^{-1} day^{-1}).	set to 0 - only required if IDFLAG = 0 - **DEVELOPMENT DEFINITION**
VHTCAP:	heat capacity per unit volume of the soil horizon (cm^{-3} $Celsius^{-1}$).	set to 0 - only required if IDFLAG = 0 - **DEVELOPMENT DEFINITION**
Record 39	**(only used for substance with metabolite)**	
DKRW12:	dissolved transformation fraction for chemical 1 to 2.	**USER INPUT** **Note:** The formation fraction of each metabolite is automatically adjusted in the shell for the molecular mass difference between metabolite and parent.
DKRW13:	dissolved transformation fraction for chemical 1 to 3.	set to 0 = not used for NCHEM = 2 - **DEVELOPMENT DEFINITION**
DKRW23:	dissolved transformation fraction for chemical 2 to 3.	set to 0 = not used for NCHEM = 2 - **DEVELOPMENT DEFINITION**
DKRS12:	sorbed transformation fraction for chemical 1 to 2.	set equal to DKRW12 - **DEVELOPMENT DEFINITION**
DKRS13:	sorbed transformation fraction for chemical 1 to 3.	set to 0 = not used for NCHEM = 2 - **DEVELOPMENT DEFINITION**
DKRS23:	sorbed transformation fraction for chemical 2 to 3.	set to 0 = not used for NCHEM = 2 - **DEVELOPMENT DEFINITION**
Record 40		
IPL:	flag to specify initial substance levels in soil before simulation start date	set to 0 = no initial conc. - **FOCUS DEFINITION**
Record 42		
ITEM1:	hydrologic hardcopy output flag	set = WATR - **DEVELOPMENT DEFINITION**
STEP1:	timestep of hydrologic output	set = YEAR - **DEVELOPMENT DEFINITION**
LFREQ1:	frequency of hydrologic output given by a specific compartment	set = 10 - **DEVELOPMENT DEFINITION**

ITEM2:	pesticide flux output flag	set = PEST - **DEVELOPMENT DEFINITION**
STEP2:	timestep of hydrologic output	set = YEAR - **DEVELOPMENT DEFINITION**
LFREQ2:	frequency of hydrologic output given by a specific compartment	set = 10 - **DEVELOPMENT DEFINITION**
ITEM3:	pesticide concentration output flag	set = CONC - **DEVELOPMENT DEFINITION**
STEP3:	timestep of hydrologic output	set = YEAR - **DEVELOPMENT DEFINITION**
LFREQ3:	frequency of hydrologic output given by a specific compartment	set = 10 - **DEVELOPMENT DEFINITION**
EXMFLG:	flag for reporting output to file for EXAMS model.	set = 0 = no EXAMS report - **DEVELOPMENT DEFINITION**
Record 45		
NPLOTS:	number of time series plots (max of 12)	set = 4 - **DEVELOPMENT DEFINITION**
STEP4:	output time step. This option output pesticide runoff and erosion flux and pesticide leaching below core depth (DAY, MNTH or YEAR)	set = DAY - **DEVELOPMENT DEFINITION**
Record 46		
PLNAME:	name of plotting variable	selected are four variables: INFL AFLX1 DFLX1 TCON1 - **DEVELOPMENT DEFINITION**
MODE:	plotting mode	set to TSER = daily - **DEVELOPMENT DEFINITION**
IARG:	argument value for PLNAME	set = 118 - **DEVELOPMENT DEFINITION**
IARG2:	argument value for PLNAME (if TSER or TCUM enter same value as IARG)	set = 118 - **DEVELOPMENT DEFINITION**
CONST:	constant with which to multiply for unit conversion.	set = 1.0 - **DEVELOPMENT DEFINITION**

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