APPENDICES

APPENDIX A . SPECIFICATION OF THE FOCUS SCENARIOS

1 FOCUS groundwater scenario for Châteaudun

Table A.1 Crop parameters for Châteaudun

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	01/04[@]	01/10[#]	4	31/05	1.9
grass + alfalfa	perennial[$]	01/04	15/05	5	15/05	0.5
		16/05	30/06	5	30/06	0.5
		01/07	15/08	5	15/08	0.5
		16/08	30/09	5	30/09	0.5
potatoes	15/04	30/04	01/09	4	15/06	0.6
sugar beets	25/03	16/04	15/10	5	15/07	1.0
winter cereals	20/10	26/10	15/07	7.5	31/05	0.8
cabbage		20/04[&]	15/07	3	31/05	0.6
		31/07[&]	15/10	3	05/09	0.6
carrots	28/02	10/03	31/05	3	20/04	0.8
	30/06	10/07	20/09	3	10/08	0.8
maize	20/04	01/05	01/10	4.5	15/08	0.8
oil seed rape (win)	30/08	07/09	10/07	4	20/04	1.0
onions	15/04	25/04	01/09	3	30/06	0.6
peas (animals)	25/03	05/04	15/08	4	07/06	0.6
spring cereals	20/02	10/03	20/07	5	10/06	0.6
tomatoes		10/05[&]	25/08	6	30/06	0.8
vines	perennial	01/04	01/11	6	31/07	1.9

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seedbed - date indicates day of transplantation.

Table A.2 Soil parameters for Châteaudun

Horizon	depth	classification	pH-H_2O*	pH-KCl†	texture µm			om	oc	bulk density	depth factor@
	cm				<2	2-50	>50	%	%	g cm^{-3}	-
Ap	0-25	silty clay loam	8.0	7.3	30	67	3	2.4	1.39	1.3	1
B1	25-50	silty clay loam	8.1	7.4	31	67	2	1.6	0.93	1.41	0.5
B2	50-60	silt loam	8.2	7.5	25	67	8	1.2	0.7	1.41	0.5
II C1	60-100	limestone#	8.5	7.8	26	44	30	0.5	0.3	1.37	0.3
II C1	100-120	limestone#	8.5	7.8	26	44	30	0.5	0.3	1.37	0
II C2	120-190	limestone#	8.5	7.8	24	38	38	0.46	0.27	1.41	0
M	190-260	limestone#	8.3	7.6	31	61	8	0.36	0.21	1.49	0

The limestone is cryoturbated in the C-horizons and powdery in the M-horizon.

* Measured at a soil solution ratio of 1:5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.

The profile is overlying an aquitanian limestone. The depth of the groundwater table is around 12 m.

Table A.3 Soil hydraulic properties, Van Genuchten/Mualem parameters (restricted form, m=1-1/n)

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

@ Plant available water in the soil layer.

Plant available water in the top 1 m is 158.6 mm.

For the MACRO model a few additional parameters are needed. These are obtained from the same original dataset. In order to avoid confusion these parameters are not included here.

2 FOCUS groundwater scenario for Hamburg

Table A4 Crop parameters for Hamburg

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2 m^{-2}$	(dd/mm)	m
apples	perennial	15/04[@]	30/10[#]	4	01/07	1.6
grass + alfalfa	perennial	25/03[$] 01/06 16/07	31/05 15/07 31/08	5 5 5	31/05 15/07 31/08	0.6 0.6 0.6
potatoes	01/05	10/05	15/09	3	20/07	0.7
sugar beets	01/04	15/04	08/10	4.2	30/08	1.2
winter cereals	12/10	01/11	10/08	3.8	01/06	1.1
beans (field)	25/03	10/04	25/08	4	10/07	0.9
cabbage		20/04[&] 31/07[&]	15/07 15/10	3 3	31/05 05/09	0.7 0.7
carrots	28/02 30/06	10/03 10/07	31/05 20/09	3 3	20/04 10/08	0.8 0.8
maize	20/04	05/05	20/09	4.2	30/07	1.2
oil seed rape (win)	25/08	02/09	28/07	4	05/05	1.1
onions	15/04	25/04	01/09	3	30/06	0.7
peas (animals)	25/03	10/04	25/08	4	10/07	0.9
spring cereals	10/03	01/04	20/08	3.9	05/06	0.9
strawberries	perennial	15/03	31/08*	2.5	30/04	0.7
vines	perennial	01/05	30/10	3	15/07	2.4

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seed bed - date indicates day of transplantation, * crop removed from field.

Table A.5 Soil texture

Horizon	depth	classification	pH-H_2O[†]	pH-KCl[*]	texture			om	oc	bulk density	depth factor[@]
	cm				<2	2-50	>50	%	%	g cm^{-3}	-
Ap	0-30	sandy loam	6.4	5.7	7.2	24.5	68.3	2.6	1.5	1.5	1.0
BvI	30-60	sandy loam	5.6	4.9	6.7	26.3	67	1.7	1	1.6	0.5
BvII	60-75	sand	5.6	4.9	0.9	2.9	96.2	0.34	0.2	1.56	0.3
Bv/Cv	75-90	sand	5.7	5	0	0.2	99.8	0	0	1.62	0.3
Cv	90-100	sand	5.5	4.8	0	0	100	0	0	1.6	0.3
Cv	100-200	sand	5.5	4.8	0	0	100	0	0	1.6	0.0

[†] These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[*] Measured at a soil solution ratio of 1:2.5

[@] The depth factor indicates the relative transformation rate in the soil layer.
Level of groundwater 2 m (estimated by IUCT).

Table A.6 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3 m^{-3}$	$m^3 m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m s^{-1}$	-	mm
						$m^3 m^{-3}$	$m^3 m^{-3}$	$*10^{-6}$		
0-30	0.3910	0.0360	1.491	1.4680	0.3188	0.292	0.064	23.330	0.500	68.4
30-60	0.3700	0.0300	1.255	1.5650	0.3610	0.277	0.047	31.670	0.500	69.0
60-75	0.3510	0.0290	1.808	1.5980	0.3742	0.229	0.040	28.330	0.500	28.4
75-90	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	21.2
90-100	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	14.1
100-200	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	

[@] AW Plant available water in the layer.
The cumulative amount over the top 1m soil is 201 mm.

3 FOCUS groundwater scenario for Jokioinen

Table A.7 Crop parameters for Jokioinen

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	10/05[@]	15/10[#]	4	25/05	1.2
grass + alfalfa	perennial[$]	15/04[$]	15/06	7	15/06	0.9
		16/06	15/07	7	15/07	0.9
		16/07	25/08	7	25/08	0.9
potatoes	15/05	05/06	25/09	5	30/08	0.6
sugar beets	10/05	25/05	15/10	5	10/08	0.9
winter cereals	10/09	20/09	15/08	4.8	25/06	0.95
bush berries	perennial	10/05	25/10	4	25/05	0.6
cabbage		20/05[&]	20/09	5	05/09	0.9
carrots	15/05	01/06	05/10	4	05/09	0.6
oil seed rape (sum)	10/05	20/05	30/08	3.8	05/07	0.8
onions	10/05	20/05	15/08	4	25/06	0.3
peas (animals)	10/05	25/05	25/08	4	30/06	0.8
spring cereals	07/05	18/05	25/08	4.5	30/06	0.8
strawberries	perennial	15/05	15/09*	2.5	25/06	0.3

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seed bed - date indicates day of transplantation, * crop removed from field.

Table A.8 Soil parameters for Jokioinen

Horizon	depth	classification	pH-H_2O*	pH-KCl†	texture µm			om	oc	bulk density	depth factor[@]
	cm				<2	2-60	>60	%	%	g cm^{-3}	-
Ap	0 - 30	loamy fine sand	6.2	5.5	3.6	23.2	73.2	7.0	4.06	1.29	1.0
Bs	30 - 60	loamy fine sand	5.6	4.9	1.8	12.2	86.0	1.45	0.84	1.52	0.5
BC1	60 - 95	loamy fine sand	5.4	4.7	1.2	14.9	83.9	0.62	0.36	1.64	0.3
BC2	95 - 100	loamy fine sand	5.4	4.7	1.7	18.9	79.4	0.50	0.29	1.63	0.3
BC2	100 - 120	loamy fine sand	5.4	4.7	1.7	18.9	79.4	0.50	0.29	1.63	0.0
Cg	120 - 150	fine sand	5.3	4.6	1.9	8.6	89.5	0.36	0.21	1.66	0.0

* Measured at a soil solution ratio of 1:2.5

† These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[@] The depth factor indicates the relative transformation rate in the soil layer.
The groundwater level is approximately 1.52 m below soil surface.

Table A.9 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-30	0.4519	0.0100	3.900	1.2745	0.2154	0.304	0.086	4.165	-0.646	65.4
30-60	0.3890	0.0100	6.650	1.4849	0.3266	0.158	0.023	5.686	-0.060	40.5
60-95	0.3632	0.0100	6.000	1.5007	0.3336	0.151	0.021	4.294	0.833	45.5
95-100	0.3636	0.0100	5.600	1.4778	0.3233	0.162	0.024	4.142	0.957	6.9
100-120	0.3636	0.0100	5.600	1.4778	0.3233	0.162	0.024	4.142	0.957	
120-150	0.3432	0.0100	7.250	1.5472	0.3537	0.121	0.017	4.834	1.036	

[@] Plant available water in soil layer.
Plant available water in top meter is 158.3 mm.

4 FOCUS groundwater scenario for Kremsmünster

Table A.10 Crop parameters for Kremsmünster

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2 m^{-2}$	(dd/mm)	m
apples	perennial	15/04[@]	30/10[#]	4	01/07	1.6
grass + alfalfa	perennial	10/04[$] 26/05 16/07	25/05 15/07 20/09	5 5 5	25/05 15/07 20/09	0.5 0.5 0.5
potatoes	01/05	10/05	15/09	3.5	20/07	0.7
sugar beets	01/04	15/04	10/10	4.2	30/08	1.2
winter cereals	25/10	05/11	10/08	4	05/06	1.1
beans (field)	25/03	10/04	25/08	4	10/07	0.8
cabbage		20/04[&] 31/07[&]	15/07 15/10	3 3	31/05 05/09	0.6 0.6
carrots	28/02 30/06	10/03 10/07	31/05 20/09	3 3	20/04 10/08	0.7 0.7
maize	20/04	05/05	20/09	4.2	30/07	1.2
oil seed rape (win)	25/08	02/09	28/07	4	05/05	1.1
onions	15/04	25/04	01/09	3	30/06	0.6
spring cereals	10/03	01/04	20/08	3.9	05/06	0.9
strawberries	perennial	15/03	31/08*	2.5	30/04	0.7
vines	perennial	01/05	30/10	3	15/07	2.4

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seed bed - date indicates day of transplantation, * crop removed from field.

Table A.11 Soil parameters for Kremsmünster

depth	classification	pH-H_2O[†]	pH-KCl[*]	texture µm			om	oc	bulk density	depth factor[@]
cm				<2	2-50	>50	%	%	g cm^{-3}	
0 - 30	loam/silt loam	7.7	7.0	14	50	36	3.6	2.1	1.41	1.0
30 - 50	loam/silt loam	7.0	6.3	25	50	25	1.0	0.6	1.42	0.5
50 - 60	loam/clay loam	7.1	6.4	27	44	29	0.5	0.3	1.43	0.5
60 - 100	loam/clay loam	7.1	6.4	27	44	29	0.5	0.3	1.43	0.3
100 - 200	loam/clay loam	7.1	6.4	27	44	29	0.5	0.3	1.43	0.0

[†] These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[*] Measured at a soil solution ratio of 1:2.5

[@] The depth factor indicates the relative transformation rate in the soil layer.

Level of groundwater (range) around 1.6 m, for apples and vines a deeper groundwater level has to be assumed. At a depth of approximately 3.3 m a rather impermeable layer is present.

Layer below 1 m copied from 60 - 100 cm layer.

Layer 0 - 30 cm is Ap horizon, 30 - 100 cm is Bwg horizon.

Table A.12 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW@
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-30	0.4246	0.0100	2.440	1.2186	0.1794	0.334	0.123	1.769	-2.080	63.3
30-50	0.4446	0.0100	2.700	1.1659	0.1423	0.365	0.169	2.780	-2.404	39.2
50-60	0.4430	0.0100	3.080	1.1578	0.1363	0.361	0.173	2.459	-2.065	18.8
60-100	0.4430	0.0100	3.080	1.1578	0.1363	0.361	0.173	2.459	-2.065	75.2
100-200	0.4430	0.0100	3.080	1.1578	0.1363	0.361	0.173	2.459	-2.065	

@ Plant available water in soil layer.
Plant available water in top meter is 196.5 mm.
Layer 100 - 200 cm copied from layer 60 - 100 cm because of lacking information.

5 FOCUS groundwater scenario for Okehampton

Table A.13 Crop parameters for Okehampton

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	m^2 m^{-2}	(dd/mm)	m
apples	perennial	25/03[@]	15/09[#]	2.5	15/06	1.5
grass + alfalfa	perennial	10/02[$] 16/05 16/07	15/05 15/07 15/09	4.5 4.5 4.5	15/05 15/07 15/09	0.45 0.45 0.45
potatoes	15/04	30/04	01/09	4	15/07	0.6
sugar beets	10/04	25/04	25/10	3	30/08	0.8
winter cereals	07/10	17/10	01/08	7.5	15/05	0.8
beans (field)	01/03	15/03	15/09	4	07/06	0.45
linseed	25/03	30/03	25/09	3	25/06	0.6
maize	07/05	25/05	07/10	7	15/07	0.8
oil seed rape (sum)	25/03	30/03	20/08	3	15/05	0.6
oil seed rape (win)	07/08	14/08	21/07	4.5	30/04	0.85
peas (animals)	25/03	05/04	15/08	4.0	07/06	0.45
spring cereals	25/03	01/04	20/08	4.5	22/05	0.6

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth.

Table A.14 Soil parameters for Okehampton

Horizon	depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
	cm				<2	2-50	>50	%	%	g cm^{-3}	(-)
A	0-25	loam	5.8	5.1	18	43	39	3.8	2.2	1.28	1.0
Bw1	25-55	loam	6.3	5.6	17	41	42	1.2	0.7	1.34	0.5
BC	55-85	sandy loam	6.5	5.8	14	31	55	0.69	0.4	1.42	0.3
C	85-100	sandy loam	6.6	5.9	9	22	69	0.17	0.1	1.47	0.3
C	100-150	sandy loam	6.6	5.9	9	22	69	0.17	0.1	1.47	0.0

[*] Measured at a soil solution ratio of 1:2.5

[†] These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[@] The depth factor indicates the relative transformation rate in the soil layer.
Level of groundwater circa 20 m.

Table A.15 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW@
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-25	0.4664	0.0100	3.550	1.1891	0.1590	0.358	0.148	3.484	-2.581	52.5
25-55	0.4602	0.0100	3.640	1.2148	0.1768	0.340	0.125	4.887	-2.060	64.5
55-85	0.4320	0.0100	4.560	1.2526	0.2017	0.290	0.090	4.838	-1.527	60.0
85-100	0.4110	0.0100	5.620	1.3384	0.2528	0.228	0.050	4.449	-0.400	26.7
100-150	0.4110	0.0100	5.620	1.3384	0.2528	0.228	0.050	4.449	-0.400	

@ Plant available water in layer.

Plant available water in top meter is 203.7 mm.

6 FOCUS groundwater scenario for Piacenza

Table A.16 Crop parameters for Piacenza

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	01/04[@]	01/11[#]	5	31/05	1.5
grass + alfalfa	perennial[$]	28/02[$] 16/05 16/07	15/05 15/07 20/09	4 4 4	15/05 15/07 20/09	0.8 0.8 0.8
potatoes	¼	20/04	10/09	5	01/06	0.5
sugar beets	01/03	20/03	15/09	4	30/06	0.8
winter cereals	25/11	01/12	01/07	7	10/05	1.0
citrus	perennial	evergreen	15/12	5	31/05	1.5
maize	30/04	15/05	30/10	5	31/07	1.0
oil seed rape (win)	30/09	05/10	20/06	3.5	15/04	0.6
soybean	25/04	10/05	05/10	6.5	31/07	0.6
sunflower	¼	20/04	20/09	4	20/06	1.0
tobacco		20/05[&]	05/10	4	20/07	1.0
tomatoes		10/05[&]	25/08	6	30/06	1.0
vines	perennial	01/04	01/11	6	31/07	2.0

[@] leaf emergence, # leaf fall, $ "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seed bed - date indicates moment of transplantation.

Table A.17 Soil parameters for Piacenza

Horizon	depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
	cm				<2	2-50	>50	%	%	$g\ cm^{-3}$	
Ap	0-30	loam	7	6.3	15	45	40	1.72	1.00	1.3	1.0
Ap	30-40	loam	7	6.3	15	45	40	1.72	1.00	1.3	0.5
Bw	40-60	silt loam	6.3	5.6	7	53	40	0.64	0.37	1.35	0.5
Bw	60-80	silt loam	6.3	5.6	7	53	40	0.64	0.37	1.35	0.3
2C	80-100	sand	6.4	5.7	0	0	100	0	0	1.45	0.3
2C	100-170	sand	6.4	5.7	0	0	100	0	0	1.45	0.0

[*] Measured at a soil solution ratio of 1:2.5

[†] These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[@] The depth factor indicates the relative transformation rate in the soil layer.

Level of groundwater 1.5 m (range 1.30-1.70 m).

Table A.18 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θs	θr	α	n	m	Water content		Ksat	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-30	0.4632	0.0100	3.050	1.2487	0.1992	0.339	0.107	4.666	-1.906	69.6
30-40	0.4632	0.0100	3.050	1.2487	0.1992	0.339	0.107	4.666	-1.906	23.2
40-60	0.4546	0.0100	2.270	1.3605	0.2650	0.317	0.063	6.217	0.316	50.8
60-80	0.4546	0.0100	2.270	1.3605	0.2650	0.317	0.063	6.217	0.316	50.8
80-100	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	28.2
100-170	0.3100	0.0150	2.812	1.6060	0.3773	0.163	0.022	28.330	0.500	

[@] Plant available water in soil layer.

Plant available water in top meter is 222.6 mm.

7 FOCUS groundwater scenario for Porto

Table A.19 Crop parameters for Porto

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2 m^{-2}$	(dd/mm)	m
apples	perennial	15/03[@]	31/10[#]	3	30/06	1.2
grass + alfalfa	perennial	28/02[$] 16/05 16/07	15/05 15/07 20/09	4 4 4	15/05 15/07 20/09	0.8 0.8 0.8
potatoes (sum)	28/02	15/03	15/06	4	30/05	0.7
sugar beets	28/02	15/03	01/08	5	30/04	1.0
winter cereals	15/11	30/11	30/6	6.5	30/04	1.0
beans (vegetable)	28/02	10/03	31/08	4	15/05	0.5
cabbage		28/02[&] 31/07[&]	01/07 15/11	4 4	15/05 31/08	0.5 0.5
carrots	15/02 15/07	28/02 22/07	31/05 15/10	4 4	01/05 15/09	0.5 0.5
citrus	perennial			6	31/05	1.5
maize	20/04	01/05	01/10	4.5	15/08	0.8
oil seed rape (sum)	15/03	22/03	25/08	3	31/05	0.9
oil seed rape (win)	30/08	07/09	10/07	4	20/04	1.0
onions	15/02	28/02	31/05	3.5	15/05	0.5
spring cereals	20/02	10/03	20/07	5	10/06	0.6
tomatoes		15/03[&]	31/08	5	15/06	0.5
vines	perennial	15/03	30/09	4	31/07	2.0

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seedbed - date indicates day of transplantation.

Table A.20 Soil texture for Porto

depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
cm				<2	2-50	>50	%	%	$g\ cm^{-3}$	-
0 - 35	loam	4.9	4.2	10	48	42	6.6	3.8	0.89	1.0
35 - 60	sandy loam	4.8	4.1	8	31	61	3.7	2.1	1.25	0.5
60 - 100	sandy loam	4.8	4.1	8	31	61	3.7	2.1	1.25	0.3
100 - 120	sandy loam	4.8	4.1	8	31	61	3.7	2.1	1.25	0.0

[*] Measured at a soil solution ratio of 1:2.5

[†] These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[@] The depth factor indicates the relative transformation rate in the soil layer.
Level of groundwater: summer lower than 2 m, winter 0.7 - 1.2 m.
Top layer is Ap horizon, other layers C1 horizon.

Table A.21 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-35	0.5780	0.0100	4.830	1.1588	0.1370	0.443	0.208	2.885	-1.630	82.25
35-60	0.4720	0.0100	4.340	1.2123	0.1751	0.339	0.125	3.142	-1.350	53.50
60-100	0.4720	0.0100	4.340	1.2123	0.1751	0.339	0.125	3.142	-1.350	85.60
100-120	0.4720	0.0100	4.340	1.2123	0.1751	0.339	0.125	3.142	-1.350	

[@] Plant available water in the soil layer.

Plant available water in top meter is 221.35 mm.

8 FOCUS groundwater scenario for Sevilla

Table A.22 Crop parameters for Sevilla

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	15/03[@]	15/10[#]	6	31/05	1.5
grass + alfalfa	perennial[$]	31/01[$]	15/04	4	15/04	0.5
		16/04	15/06	4	15/06	0.5
		16/06	15/08	4	15/08	0.5
		16/08	15/10	4	15/10	0.5
potatoes	15/01	31/01	31/05	4	31/03	0.5
sugar beets	31/10	10/11	01/07	5	15/04	0.6
winter cereals	15/11	30/11	31/05	7	28/02	0.40
cabbage		01/03[&]	01/06	3	01/05	0.5
		15/06[&]	15/09	3	15/08	0.5
citrus	evergreen			6	31/05	1.5
cotton	25/03	05/04	31/07	5	30/04	0.6
maize	28/02	07/03	31/07	6	15/06	0.4
strawberries	perennial	30/11[&]	31/08[*]	3	30/04	0.25
sunflower	01/03	10/03	15/07	4	15/06	0.60
tomatoes		15/04[&]	01/07	6	30/05	0.8
vines	perennial	31/03	30/11	5	15/06	1.5

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] transplanted from seed bed - date indicates day of transplantation.

Table A.23 Soil parameters for Sevilla

depth	classification	pH-H_2O[*]	pH-KCl[†]	texture µm			om	oc	bulk density	depth factor[@]
cm				<2	2-50	>50	%	%	$g\ cm^{-3}$	-
0-10	silt loam	7.3	6.6	14	51	35	1.6	0.93	1.21	1.0
10-30	silt loam	7.3	6.6	13	52	35	1.6	0.93	1.23	1.0
30-60	silt loam	7.8	7.1	15	51	34	1.2	0.70	1.25	0.5
60-100	clay loam	8.1	7.4	16	54	30	1.0	0.58	1.27	0.3
100-120	clay loam	8.1	7.4	16	54	30	1.0	0.58	1.27	0.0
120-180	clay loam	8.2	7.5	22	57	21	0.85	0.49	1.27	0.0

[*] Measured at a soil solution ratio of 1:2.5

[†] These values are estimated from the measured water values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

@ The depth factor indicates the relative transformation rate in the soil layer.
The groundwater level is approximately 2.4 m below soil surface. If necessary the bottom soil layer can be extended to this depth.

Table A.24 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θs	θr	α	n	m	Water content		Ksat	λ	AW[@]
cm	$m^3 m^{-3}$	$m^3 m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m s^{-1}$	-	mm
						$m^3 m^{-3}$	$m^3 m^{-3}$	$*10^{-6}$		
0-10	0.4904	0.0100	2.500	1.2688	0.2119	0.364	0.106	4.819	-1.496	25.8
10-30	0.4836	0.0100	2.450	1.2767	0.2167	0.358	0.101	4.362	-1.374	51.4
30-60	0.4798	0.0100	2.500	1.2695	0.2123	0.356	0.104	4.596	-1.465	75.6
60-100	0.4747	0.0100	2.360	1.2673	0.2109	0.357	0.105	3.911	-1.423	100.8
100-120	0.4747	0.0100	2.360	1.2673	0.2109	0.357	0.105	3.911	-1.423	
120-180	0.4795	0.0100	2.280	1.2297	0.1868	0.377	0.131	3.350	-1.858	

@ Plant available water in soil layer
Plant available water in top meter is 253.6 mm.

9 FOCUS groundwater scenario for Thiva

Table A.25 Crop parameters for Thiva

Crop	Growth stage			LAI and interception		Root depth
	Planting	Emergence	Harvest	Max. LAI		
	(dd/mm)	(dd/mm)	(dd/mm)	$m^2\ m^{-2}$	(dd/mm)	m
apples	perennial	15/03[@]	20/10[#]	5	30/06	1.5
grass + alfalfa	perennial	15/04[$]	30/06	4	30/06	0.6
		01/07	15/08	4	15/08	0.6
		16/08	30/09	4	30/09	0.6
		01/10	15/11	4	15/11	0.6
potatoes	15/02	01/03	30/07	4	30/04	0.6
sugar beets	15/04	01/05	30/09	5	30/06	0.9
winter cereals	15/11	30/11	30/06	7.5	30/03	0.8
beans (vegetables)	25/03	01/04	15/06	4	01/05	0.6
	01/07	08/07	30/9	4	08/08	0.6
cabbage		15/08[&]	30/11	4	30/09	0.6
carrots	01/03	15/03	22/05	4	15/04	0.6
	01/06	15/06	10/09	4	15/07	0.6
citrus	perennial		30/11	5		1.5
cotton	01/05	15/05	30/08	5	15/07	0.8
maize	01/04	20/04	15/09	4.5	15/06	0.8
onions	15/02	10/04	30/06	4	15/06	0.6
tobacco		01/05[&]	30/09	5	15/08	0.6
tomatoes	na	10/04[&]	10/09	4	30/05	0.6
vines	perennial	15/03	20/10	4	30/06	2.0

[@] leaf emergence, [#] leaf fall, [$] "harvest" and "emergence" dates represent the cutting and subsequent regrowth, and so affect above ground biomass but not rooting depth, [&] crops are transplanted from seed beds - in the column emergence the date of transplantation is given.

Table A.26 Soil texture

Horizon	depth	classification	pH-H_2O[†]	pH-KCl[*]	texture			%om	%oc	bulk density	depth factor
					<2	2-50	>50	%	%	g cm^{-3}	-
Ap1	0-30	loam	7.7	7.0	25.3	42.8	31.9	1.28	0.74	1.42	1.0
Ap2	30-45	loam	7.7	7.0	25.3	42.8	31.9	1.28	0.74	1.42	0.5
Bw	45-60	clay loam	7.8	7.1	29.6	38.7	31.7	0.98	0.57	1.43	0.5
Bw	60-85	clay loam	7.8	7.1	31.9	35.7	32.3	0.53	0.31	1.48	0.3
Ck1	85-100	clay loam	7.8	7.1	32.9	35.6	31.5	0.31	0.18	1.56	0.3
Ck1	100-???	clay loam	7.8	7.1	32.9	35.6	31.5	0.31	0.18	1.56	0.0

[†] These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

[*] Measured at a soil solution ratio of 1:2.5

[@] The depth factor indicates the relative transformation rate in the soil layer.
Level of groundwater > 5 m.

Table A.27 Soil hydraulic properties, Van Genuchten/Mualem parameters

depth	θ_s	θ_r	α	n	m	Water content		K_{sat}	λ	AW[@]
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	10kPa	1600kPa	$m\ s^{-1}$	-	mm
						$m^3\ m^{-3}$	$m^3\ m^{-3}$	$*10^{-6}$		
0-30	0.4341	0.01	3.33	1.1804	0.15283	0.340	0.147	3.48	-3.162	58.02
30-45	0.4341	0.01	3.33	1.1804	0.15283	0.340	0.147	3.48	-3.162	29.01
45-60	0.4412	0.01	3.58	1.1330	0.117387	0.365	0.196	2.28	-3.402	25.43
60-85	0.4279	0.01	3.62	1.1252	0.111269	0.357	0.199	1.83	-3.312	39.70
85-100	0.4041	0.01	3.37	1.1145	0.102737	0.345	0.202	1.26	-3.259	21.44
100-???	0.4041	0.01	3.37	1.1145	0.102737	0.345	0.202	1.26	-3.259	

[@] Plant available water in the soil layer.

Plant available water in top meter soil is 142.9 mm.

Layer 100 - ??? cm copied from layer 85 - 100 cm; this layer can be extended according to the needs of the models.

10 Reference

Barrere, C., Bastide, J., Coste, C.M. 1988. Relations entre la vitesse de degradation du propyzamide et les proprietes physicochimique des sols. Weed research **28**, pp93 - 99.

APPENDIX B . PARAMETERISATION OF MACRO

1 Introduction

For the MACRO model, the parameters are given under different headings in a menu-based system. The following sections follow each of these headings systematically. MACRO was parameterised for Châteaudun only in relation to the FOCUS groundwater scenarios.

A common shell program has been written for the MACRO model (version 4.2) to run the single FOCUS groundwater scenario (Châteaudun) as well as the six FOCUS surface water scenarios developed for MACRO. The shell program is PC-based and written in Visual Basic. All parameter values defining the scenarios are contained in a number of Microsoft Access databases. For the single groundwater scenario at Châteaudun, the user simply selects a crop from the available list, and then sets options for the length of simulation (20, 40 or 60 years), and whether or not macropore flow and irrigation are to be simulated (in the latter case, for those crops which may be irrigated). Substance properties can also be defined interactively and stored in a separate database for later use. In-built calculation and plot routines present the results of the simulations to the user in the correct format for FOCUS, both in tables and figures.

The implemented scenario and parameter definitions are based on:

- **FOCUS DEFINITION** = Definitions made by the FOCUS working group
- **FOCUS SCENARIO SPECIFIC** = Definitions made by the FOCUS working group for a specific scenario
- **DEVELOPMENT DEFINITION** = Definitions made during the MACRO file development
- **USER INPUT** = Input to be specified by the user in the MACRO shell

2 Input files

The meteorological files are entered as bin-files. They contain the following information:

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

In addition, a parameter file has to be specified (.par). The choice will depend on the crop selected for the simulation. The input present in the parameter file is described below. For metabolites, an output file from the simulation of the mother substance is required.

3 Switches

Technical

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

Model Specific

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

4 Parameters

Soil profile

<table>
<tr><th colspan="2"><u>Parameter and description</u></th><th><u>Value, source & comments</u></th></tr>
<tr><td>Nlayer</td><td>Number of layers to be simulated (max 15)</td><td>Set to 15 -DEVELOPMENT DEFINITION</td></tr>
<tr><td>Z(1-15)</td><td>Depth in mm of the 15 layers</td><td>The division between the layers is chosen on the basis that
i) a horizon should preferably contain at least 3 layers,
ii) the top horizons should be below 5 cm,
iii) to avoid numerical dispersion, the layers should not exceed 10 cm,
iv) the division between layers should equal the division between horizons
v) below 1 m, an attempt was made to extend the depth as much as possible (violating criteria iii above)
The fact that the layers are greater than 10 cm below 1 m depth means that dispersion is overestimated. This will overestimate leaching to depths greater than 1 m. Despite this, results up to 1.9 m depth are considered acceptable at a higher tier, because the additional dispersion is conservative in its effect. More layers will be allowed in the next version of MACRO, expected during 2000. (DEVELOPMENT DEFINITION)
The final division at Châteaudun was
<table>
<tr><td>Horizon</td><td>Layers, mm</td><td>Final depth, cm</td></tr>
<tr><td>1</td><td>20+60+80+90</td><td>25</td></tr>
<tr><td>2</td><td>80+90+80</td><td>50</td></tr>
<tr><td>3</td><td>100</td><td>60</td></tr>
<tr><td>4</td><td>100+100+100+100</td><td>100</td></tr>
<tr><td>5</td><td>200</td><td>120</td></tr>
<tr><td>6</td><td>300+400</td><td>190</td></tr>
</table>
</td></tr>
</table>

Site

Parameter and description		Value, source & comments
ANNAMP	The temperature amplitude between the average temperature in January and July. (°C)	Calculated from the weather record to be 7.7°C. **FOCUS SCENARIO SPECIFIC**.
ANNTAV	The average annual temperature (°C)	Calculated from the weather record to be 11.9°C. **FOCUS SCENARIO SPECIFIC**.
PHI	Site latitude	**FOCUS SCENARIO SPECIFIC**
RAINCO	Correction coefficient for rain.	For the scenarios it is assumed to be 1. **DEVELOPMENT DEFINITION**
RINTEN	A typical rainfall intensity for the area in question (mm hr^{-1}).	For southern England, a value of 2 mm/hr is realistic. The same value was selected for Châteaudun. **DEVELOPMENT DEFINITION**
SNOWCO	Correction factor for snowfall.	For the scenarios it is assumed to be 1. **DEVELOPMENT DEFINITION.**
SNOWMF	The factor governs the rates of snowmelt,	Set to default, 4.5 mm $degree^{-1}$ day^{-1}. Snow is not regarded to be important in Châteaudun. **DEVELOPMENT DEFINITION**.

Initial/Boundary conditions

Parameter and description		Value, source & comments
BOTEN	Tension at the lower boundary of the profile (cm)	For groundwater in 12 m's depth as defined for Châteaudun, the value is calculated as (190 cm – 1200 cm = -1010 cm). The resulting tension at the bottom of the soil column is 1010 cm. **DEVELOPMENT DEFINITION** based on **FOCUS SCENARIO SPECIFIC** parameters.
CONCIN	Solute concentration at the bottom boundary	Set to zero (**FOCUS DEFINITION**)
SOILINIT	Initial concentration in the soil	Set to zero (**FOCUS DEFINITION**)
TEMPINI	Initial temperature in the soil profile.	Set to 10°C. Due to the warming up period, the initial values are without importance for the simulation. **DEVELOPMENT DEFINITION**.

Solute transport

Parameter and description		Value, source & comments
AEXC	Excluded volumetric water content due to anion exclusion. (%)	Set to 0. **DEVELOPMENT DEFINITION**.
CONC	The solute concentration in rainfall	Set to zero. **FOCUS DEFINITION**
DIFF	The diffusion coefficient for the substance (m^2 s^{-1})	**USER INPUT**. The default value is 5.0 E-10.
DV	Dispersivity (cm)	Set to 5 cm – **FOCUS DEFINITION**
FSTAR	The solute concentration factor for crop uptake of substance	**USER INPUT**. The default value is 0.5
ZMIX	Mixing depth for rainfall and soil moisture (mm).	Set to 1 mm (default). **DEVELOPMENT DEFINITION**.

Substance

Parameter and description		Value, source & comments
CANDEG	Degradation on leaves	The default value is 0.2. The factor only ensures that substance on the leaves degrade fast. As the substance by **FOCUS DEFINITION** cannot wash off the leaves, the value does not influence leaching.
DEGMAL	Degradation factor (ln2/half life in days), at a moisture content of XMPOR and the temperature TREF, for the liquid phase in the macropores	**USER INPUT**, for each of the 15 layers. Although MACRO internally uses XMPOR as the reference moisture for degradation, it has been ensured through the shell that the degradation value at pF2 is exactly equal to that which is used in the other FOCUS models.
DEGMAS	As above, for the solid phase in the macropores	**USER INPUT**, for each of the 15 layers.
DEGMIL	As above, for the liquid phase in the micropores.	**USER INPUT**, for each of the 15 layers.
DEGMIS	As above, for the solid phase of the micropores.	**USER INPUT**, for each of the 15 layers.
		In general, the four values above have to be corrected for the moisture content. Unless other information is available, the four values for a given depth may be identical.
EXPB	Exponent of moisture corrected degradation (moisture relationship according to WALKER)	0.7 (default value)
FCONVERT	Fraction of degraded parent compound converted to metabolite.	**USER INPUT**.
FEXT	Wash-off coefficient for the leaves.	Set to 0. This ensures that substance sprayed onto the leaves will not enter the leaching calculation. **FOCUS DEFINITION**.
FRACMAC	The ratio of macropores to total porosity	The value was calculated as 0.028 in the upper m of the Châteaudun profile. The default value of 0.02 was kept, as it is expected that the adsorption sites are less well used due to the high velocity of water in the macropores. **DEVELOPMENT DEFINITION**.
FREUND	Exponent of the Freundlich isotherm	**USER INPUT**
TREF	Reference temperature for substance degradation value (Celsius)	**USER INPUT**
TRESP	Exponent in the temperature response function ($Kelvin^{-1}$)	0.079 (default value)
ZKD	Sorption distribution coefficient, $cm^3 g^{-1}$ (Kd)	**USER INPUT**

Physical/Hydraulic properties

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

Parameter and description		Value, source & comments
ASCALE	Effective diffusion path length (aggregate half width), mm	Determined via the transfer functions in MACRO_DB, based on the description of soil structure. The values of ASCALE chosen are 10 (0-25 cm), 75 (25-60 cm), 1 (60-120 cm) and 4 (120-190 cm). **DEVELOPMENT DEFINITION**
CTEN	Tension of the saturated micro-pores = boundary soil water tension, cm.	**DEVELOPMENT DEFINITION** The value may be identified from measured unsaturated hydraulic conductivity curves, as the place where the curve „breaks“. The Villamblain data did not cover the tension range close to saturation. The values were chosen to give 1) a good fit to the unsaturated conductivity, with 2) a value as close to saturation as possible (if CTEN moves too far away from saturation, the model assumption of gravity flow in macropores breaks down. The value is given as h_B in the Table B.2.
GAMMA	Bulk density (g/cm^3)	**FOCUS SCENARIO SPECIFIC**
KSATMIN	The saturated hydraulic conductivity (mm hr^{-1})	Given in Table B.1 as Ksat for Châteaudun. **FOCUS SCENARIO SPECIFIC**.
KSM	The hydraulic conductivity for the micropores, at a tension value of CTEN (mm hr^{-1})	Set to K_b in Table B.2. **DEVELOPMENT DEFINITION**
RESID	Residual moisture content, %	Given in Table B.1 as θ_r for Châteaudun. **FOCUS SCENARIO SPECIFIC**.
TPORV	Saturated water content, %	Given in Table B.1 as θ_s for Châteaudun. **FOCUS SCENARIO SPECIFIC**.
WILT	Wilting point, %	**FOCUS SCENARIO SPECIFIC**, but slightly changed due to the fact that MACRO requires Brooks Corey-parameters. Given in Table B.2 as water content at 1600kPa for Châteaudun.
XMPOR	Boundary soil water content, %	Set to θ_b from Table B.2. **DEVELOPMENT DEFINITION**.
ZA	Parameter relevant for simulation of shrinkage	Set to 1. Irrelevant for the simulation
ZLAMB	Pore size distribution index	Set to b in Table B.2. **DEVELOPMENT DEFINITION**
ZM	Tortuosity factor, micropores	Set to lambda in Table B.2. **DEVELOPMENT DEFINITION**.
ZN	Tortuosity factor, macropores	The value of ZN was chosen based on a very approximate calibration against measured water discharges from the Villamblain lysimeters. A value of 3.0 is selected down to 60 cm, 2 in the deeper layers. **DEVELOPMENT DEFINITION**
ZP	Indicates presence or absence of shrinkage	Set to 0 = no shrinkage. **DEVELOPMENT DEFINITION**.

Crop

A table of crop parameters for the crops at Châteaudun has been attached as Table B.3.

Parameter and description		Value, source & comments
BETA	Root adaptability factor	**DEVELOPMENT DEFINITION** for each crop (and site).
CANCAP	Maximum water interception by the crop, mm	CANCAP may be calculated as approximately 0.5 * LAI max. However, values were selected to match the FOCUS surface water scenarios. **DEVELOPMENT DEFINITION**.
CFORM	Form factor for the period from emergence to maturity	The values given in Table B.3 are derived from visual comparisons between published growth curves and fitted curves. **DEVELOPMENT DEFINITION**.
CRITAIR	Critical soil air content for root water uptake, %	Kept at Default =5. This value is not too far from the difference between field capacity and saturation weighted through the first meter of the profile, and also the default value used for the FOCUS surface water group. **DEVELOPMENT DEFINITION**.
DFORM	Form factor for the period from maturity to harvest	The values given in Table B.3 are derived from visual comparisons between published growth curves and fitted curves. **DEVELOPMENT DEFINITION**.
IDMAX	The day of maturity of the crop	**FOCUS SCENARIO SPECIFIC**
IDSTART	The day of emergence of the crop	**FOCUS SCENARIO SPECIFIC**
IDHARV	The day of harvest of the crop	**FOCUS SCENARIO SPECIFIC**
LAIHARV	LAI at harvest	The values given in Table B.3 are derived from visual interpretation of published growth curves. **DEVELOPMENT DEFINITION**
LAIMAX	LAI at maturity	**FOCUS SCENARIO SPECIFIC**
LAIMIN	The LAI at the date ZDATEMIN	For summer crops the value is close to 0, for winter crops it is the LAI value during early spring. **DEVELOPMENT DEFINITION**.
ROOTINIT	The root depth at the date ZDATEMIN, m.	Set to the values given in Table B.3. For summer crops the value is close to 0, for winter crops it is the root depth during early spring. **DEVELOPMENT DEFINITION**.
ROOTMAX	Maximum root depth, m.	**FOCUS SCENARIO SPECIFIC**.
RPIN	Percentage of the root length in the top 25 % of the root depth.	Set to 60 % (Default). **DEVELOPMENT DEFINITION**.
WATEN	Critical tension for root water uptake, m	Set to 10 m (Default). **DEVELOPMENT DEFINITION**.
ZALP	Correction factor for evaporation from wet canopy.	Given in Table B.3 and B.4 for the different crops. **FOCUS SCENARIO SPECIFIC**.
ZDATEMIN	The day number corresponding at LAIMIN, ROOTINIT and ZHMIN	Values given in Table B.3, set one day after emergence for summer crops and as 90 days for the winter crops. The growth is expected to increase significantly after this date. **DEVELOPMENT DEFINITION**.
ZHMIN	The crop height at the date ZDATEMIN	Values given in Table B.3. For summer crops the value is close to 0, for winter crops it is the height during early spring. **DEVELOPMENT DEFINITION**.

Irrigation

Parameter and description		Value, source & comments
AMIR	Amount of irrigation water applied, mm, in which the substance is mixed.	**USER INPUT** 1000 l/ha = 1 m^3/10,000 m^2 = 0.1 mm is often used due to ease of calculation
CONCI	Concentration of the substance in the irrigation water, mg m^{-3}	**USER INPUT** Example: 1 kg/m^3= 1,000,000 mg/m^3
CRITDEF	Specification of criteria for irrigation	As there is no automatic irrigation, the value should be set to (-1). **DEVELOPMENT DEFINITION**
IRRDAY	Day of irrigation (Day of substance application)	**USER INPUT**
IRREND	Time when the irrigation ends.	Given as hours and minutes as decimal fraction. Set to 9.2: **DEVELOPMENT DEFINITION**
IRRSTART	Time when the irrigation starts	Given as hours and minutes as decimal fraction. Set to 9. **DEVELOPMENT DEFINITION**
NIRR	Number ofirrigations	**USER INPUT**
ZFINT	The fraction of the substance which is intercepted	**USER INPUT**. The fraction of interception is selected according to the interception table as described in the guidelines for parameter selection. It is also possible to calculate manually the amount of pesticide reaching the ground, and use this as the basis for the input concentration (CONCI). In this case ZFINT is set to 0. This solution is recommended for the other models.

5 Output specification

The minimum output specification requirements are the following: Parameters are specified to allow calculation of a water-balance for a 1 m profile and for the full profile, as well as for analysing the parameters for registration purposes. Daily values of each variable are reported, see Section 6.

Miscellaneous (water)

Parameter and description		Value, source & comments
THETT	Total water content, micropores and macropores, $m^3 m^{-3}$	Should be specified at least for the upper m of the horizon (=1-12)
WFLOWOUT	Water flow rate out of layer from macropores, mm h^{-1}	Should be specified at least for layer 12, the output depth
WOUT	Water flow rate out of layer from micropores, mm h^{-1}	Should be specified at least for layer 12, the output depth

Water balance

Parameter and description		Value, source & comments
CETA	Actual evapotranspiration rate, mm hr^{-1}	This parameter, or the next may be used for deriving the yearly actual evaporation.
CCET	Accumulated actual evapotranspiration, mm	
PRECIRRr	Precipitation and irrigation rate, mm hr^{-1}	This parameter, or the next may be used for deriving the yearly actual evaporation..
PRECIRA	Accumulated precipitation and irrigation rate, mm	
SRUNOFF	Runoff, mm hr^{-1}.	This parameter, or the next may be used for deriving the yearly surface runoff.
TRUNOFF	Accumulated surface runoff, mm	
TSTOREMI	Total water storage in micropores through the whole profile, mm	The figure relates to the full profile and not the water balance at 1 m depth.
TSTOREMA	Total water storage in macropores through the whole profile, mm	The figure relates to the full profile and not the water balance at 1 m depth.
TFLOWOUT	Total accumulated percolation, mm (micropores and macropores)	The figure relates to the bottom of the profile, and not to the water balance at 1m depth.

Miscellaneous, other

Parameter and description		Value, source & comments
DEGMAC	Solute degraded in soil macropores, mass m^{-2} h^{-1}	Should be indicated at least for the upper m (=1-12)
DEGMIC	Solute degraded in soil micropores, mass m^{-2} h^{-1}	Should be indicated at least for the upper m (=1-12)
SFLOW	Solute flow rate out of layer, micropores, mass*m^{-2}*h^{-1}	Should be indicated at least for the result layer (12)
SFLOWOUT	Solute flow rate out of layer, macropores, mass*m^{-2}*h^{-1}	Should be indicated at least for the result layer (12)
SOLMAC	Solute concentration in macropores, mass m^{-3}	Should be indicated at least for the upper m (=1-12)
SOLMIC	Solute concentration in micropores, mass m^{-3}	Should be indicated at least for the upper m (=1-12)
SMACIN	Solute infiltration, macropores, accumulated, mass m^{-2}	Together with the next output variable, it specifies the substance input
SMICIN	Solute infiltration, micropores, accumulated, mass m^{-2}	See SMACIN above

Solute balance

Parameter and description		Value, source & comments
ADMA	Solute stored in macropores in solid form (sorbed)	Should be indicated at least for the upper m (=1-12)
ADMI	Solute stored in micropores in solid form (sorbed)	Should be indicated at least for the upper m (=1-12)
CAM	Solute stored in macropores in the liquid phase	Should be indicated at least for the upper m (=1-12)
PAM	Solute stored in micropores in the liquid phase	Should be indicated at least for the upper m (=1-12)
PCAA	Total solute storage, mass m^{-2}	If the user is interested in the total storage only, this output could be specified instead of ADMA, ADMI, CAM and PAM.
TADMA	Solute storage in profile, macropores only, solid phase, mass m^{-2}	
TADMI	Solute storage in profile, micropores only, solid phase, mass m^{-2}	
TDEG	Accumulated total degradation in the soil, mass m^{-2}	For this parameter, the value for the upper meter and for the profile is identical, due to the fact that degradation is specified for the upper meter only.
TSUPT	Accumulated uptake of solute by crop, mass m^{-2}	If the root depth is less than one meter, the value for the profile is identical to the value for the upper meter.
TCAM	Solute storage in macropores in the liquid phase, for the profile	
TPAM	Solute storage in micropores in the liquid phase for the profile	
TSOUT	Accumulated solute leaching (total for macro- and micropores), mass m^{-2}	
TSRUN	Accumulated amount of solute lost in runoff, mass m^{-2}	

6 Run specification

The run specification should be daily outputs, with user start time 1901 01 01 and user specified end time.

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

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

@ Plant available water in the soil layer.

Plant available water in the top 1 m is 158.6 mm.

Table B.2 Soil hydraulic properties, Brooks-Corey/Mualem parameters (as used in the MACRO model)

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

Note: Ksat and θ_s are the same as for the Mualem/van Genuchten fit shown in Table B.1.

@ Plant available water in the soil layer.

Plant available water in the top 1 m is 150.3 mm.

Table B.3 Parameters for the FOCUS crops for Châteaudun.

	Crop										
Parameter	**potatoes**	**sugar beet**	**cabbage**	**carrots**	**maize**	**0nion**	**peas**	**spring cereals**	**tomatoes ***	**winter cereals**	**oil seed rape (w)**
Crop	2	2	2	2	2	2	2	2	2	2	2
CHAPAR			on	on							
Date			197	180							
BETA	0.5	0.2	0.5	0.5	0.2	0.5	0.5	0.2	0.5	0.1	0.1
CanCap	2	2.5	2	2	3	2	2	2	2	3	3
Cform	1.7	1.7	1.5	1.5	1.7	1.5	1.7	2	1.3	2	2
Critair	5	5	5	5	5	5	5	5	5	5	5
D-form	0.3	1	1	1	0.3	1	0.3	0.3	0.3	0.2	0.2
IDMax	166	196	151/248	110/222	227	181	158	161	181	151	110
IDStart	120	106	110/212	69/191	121	115	95	69	130	299	250
Iharv	244	288	196/288	151/263	274	244	227	201	237	196	191
LAIHAR	2	5	3	3	2	3	3	2	3	2	2
LAIMAX	4	5	3	3	4.5	3	4	5	6	7.5	4
LAIMIN	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.3	1	1
Rootinit	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.1	0.2	0.2
Rootmax	0.6	1	0.6	0.8	0.8	0.6	0.6	0.6	0.8	0.8	1
RPIN	75	67	75	75	67	75	67	60	67	60	60
WATEN	10	20	10	10	20	10	10	20	10	50	50
ZALP	1	1	1	1	1.5	1	1	1	1	1	1
ZDATEMIN	121	107	111/213	70/192	122	116	96	70	131	90	90
ZHMIN	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.1	0.2	0.2

Table B.4 Crop parameters for perennial crops.

	Crop			
Parameter	**apples**	**wine**	**grass + alfalfa**	
Crop	2	2	3	
CHAPAR				
Date				
BETA	0.2	0.2	0.2	
CanCap	4	3	2	
Cform	1.5	1.5		
Critair	5	5	5	
D-form	0.7	0.7		
IDMax	151	212		
IDStart	91	91		
Iharv	274	305		
LAIHAR	0.01	0.01		
LAIMAX	4	6	5	(LAIC)
LAIMIN	0.01	0.01		
Rootinit	1.89	1.89		
Rootmax	1.9	1.9	0.5	
RPIN	60	60	67	
WATEN	20	20	20	
ZALP	3	2	1	
ZDATEMIN	92	92		
ZHMIN	4.99	1.79		
HCROP	5	1.8	0.2	

Table B.5 Properties for the dummy substances A, B, C and its metabolite, and D

	Substance					Comments	
parameter	**A**	**B**	**C**	**metabolite**	**D**		
Metabolite	off	off	on	off	off		
Driving	0	0	0	1	0	The metabolite is run with the output file from C as input	
Solute	2	2	2	2	2		
AEXC	0	0	0	0	0		
Conc	0	0	0	0	0		
DIFF	5.00E-10	5.00E-10	5.00E-10	5.00E-10	5.00E-10		
DV	5	5	5	5	5		
Fstar	0.5	0.5	0.5	0.5	0.5		
Zmix	1	1	1	1	1		
Candeg	0.2	0.2	0.2	0.2	0.2	Only effect to make substance on leaves disappear.	
Degmal(1-4)	0.0125	0.0375	0.0375	0.00750	0.0375	Degmas, Degmil, and Degmis receive the same values	
Degmal(5-8)	0.00639	0.01918	0.01918	0.00385	0.01918		
Degmal(9-12)	0.00379	0.01137	0.01137	0.00228	0.01137		
Degmal(13-15)	0	0	0	0	0		
EXPB	0.7	0.7	0.7	0.7	0.7		
FEXT	0	0	0	0	0		
FCONVERT				0.53			
FRACMAX	0.02	0.02	0.02	0.02	0.02		Dosage for all substances is 1 kg/ha
FREUND	0.9	0.9	0.9	0.9	0.9		applied on day 69 between 6 and 6.5 am
TREF	20	20	20	20	20		AMIR = 0.1, conci = 1E6 mg/m3.
TRESP	0.079	0.079	0.079	0.079	0.079		
ZKD(1-4)	1.41	0.233	2.36	0.712	0.82		
ZKD(5-7)	0.95	0.156	1.58	0.478	0.551		
ZKD(8)	0.72	0.119	1.2	0.364	0.418		
ZKD(9-13)	0.31	0.051	0.516	0.156	0.18		
ZKD(14-15)	0.28	0.046	0.464	0.14	0.162		
ZFINT	0	0	0	0	0		

7 References

Jarvis N, 1994. The MACRO Model (Version 3.1). Technical Description and Sample Simulations. Department of Soil Sciences, Swedish University of Agricultural Sciences. Reports and Dissertations, 19. Uppsala 1994.

APPENDIX C . PARAMETERISATION OF PELMO

1 Introduction

The PELMO version that was used for the implementation of the FOCUS-scenarios was developed in 1999 (PELMO 3.2). It was necessary to change the format of the scenario and pesticide data files and the handling of leap years slightly because of the needs of the FOCUS-scenarios. Minor changes were also made in the routine that is estimating soil temperatures based on air temperatures to make sure that the results are correct also for soil depths below 1.0 m. Finally, the runoff routine in PELMO was calibrated based on field experiments by introducing a new parameter in the model ("fraction of soil water available for runoff").

2 Description of the PELMO shell

PELMO.EXE runs under Microsoft DOS. However, to make editing and creating of PELMO input files easier in a Microsoft Windows environment, a shell called WPELMO.EXE was built around PELMO.EXE.

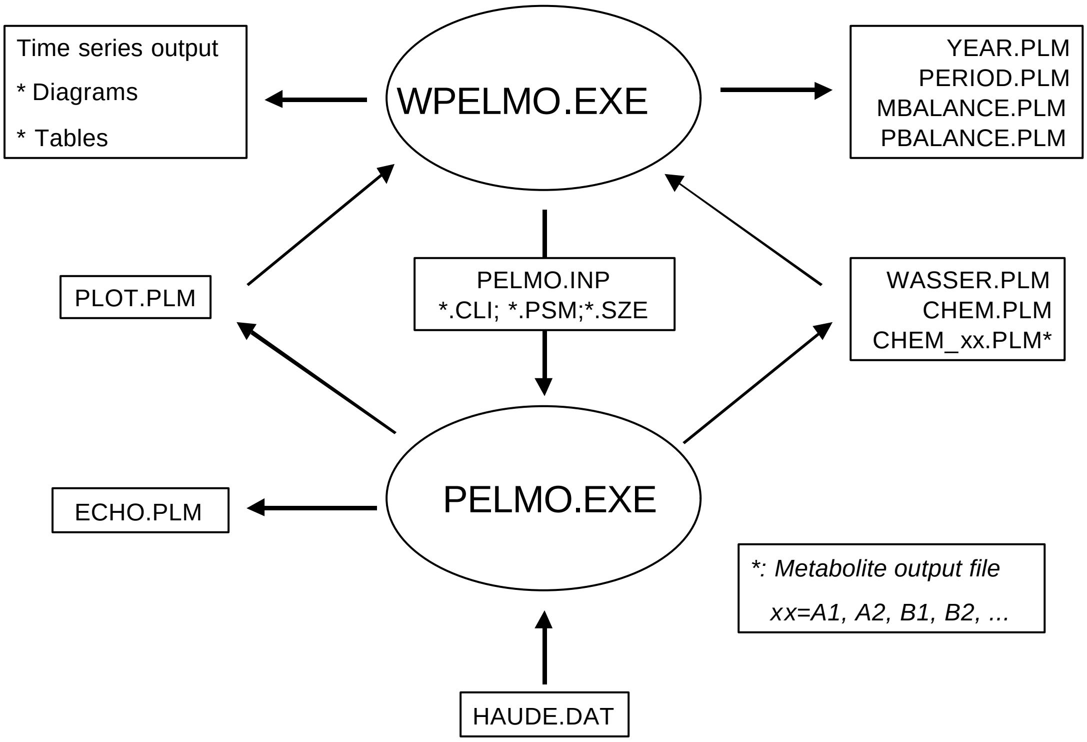
File handling

The information necessary to run PELMO.EXE is divided in a number of input data files. The shell WPELMO.EXE allows creating or editing of these files by the user. For each simulation a single substance data file (extension: PSM), a single scenario data file (extension: SZE) and a number of climate data files (extension: CLI) are necessary. For FOCUS-tier 1 -simulations only the substance data file has to be created by the user himself; the scenario and climate data files are already defined and should not be modified.

Before the user starts a PELMO simulation the scenario (location and crop, possibly irrigation) and the substance data file has to be set. The required scenario and climate input data files (*.cli and *.sze) are automatically selected by the shell and written into a small ASCII file called PELMO.INP. This file will be read by the simulation program PELMO.EXE (see Figure C.1).

The file HAUDE.DAT contains the monthly Haude-factors. This information is not used for FOCUS-simulations. However, the file must be in the FOCUS-directory of PELMO.

Figure C.1 File handling between the simulation program PELMO.EXE and the shell WPELMO.EXE



During the simulation PELMO.EXE creates a number of output files:

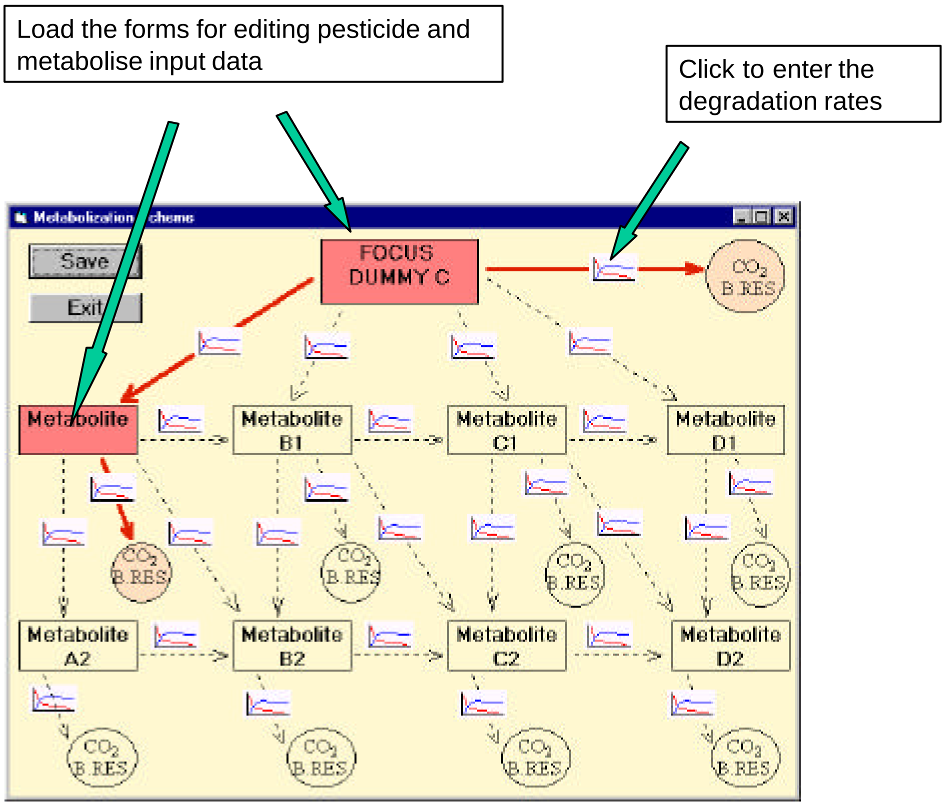
- ECHO.PLM: echo of all input parameters of the specific simulation
- WASSER.PLM: hydrologic output data (tables)
- CHEM.PLM: substance output data (tables)
- CHEM_xx: metabolite output data (tables), xx=A1, A2, B1, B2, ...
- PLOT.PLM: time series output file, used by WPELMO.EXE to create diagrams

After a PELMO simulation has been successfully performed the annual average concentrations at 1 m depth and at the soil bottom are calculated by WPELMO.EXE based on the results stored in WASSER.PLM (hydrology output), CHEM.PLM (substance output) and CHEM_xx (metabolite output). WPELMO also creates the files MBALANCE.PLM and PBALANCE.PLM that contain the total annual mass balances for water (MPBALANCE:PLM) and for the substance/metabolites (PBALANCE.PLM).
WPELMO.EXE allows archiving of simulations. If the user would like to store the results of PELMO simulations the output data files will be moved into the directory ARCHIVE using an individual extension (number between 000 and 999 instead of PLM).

Creating substance data files for PELMO simulations

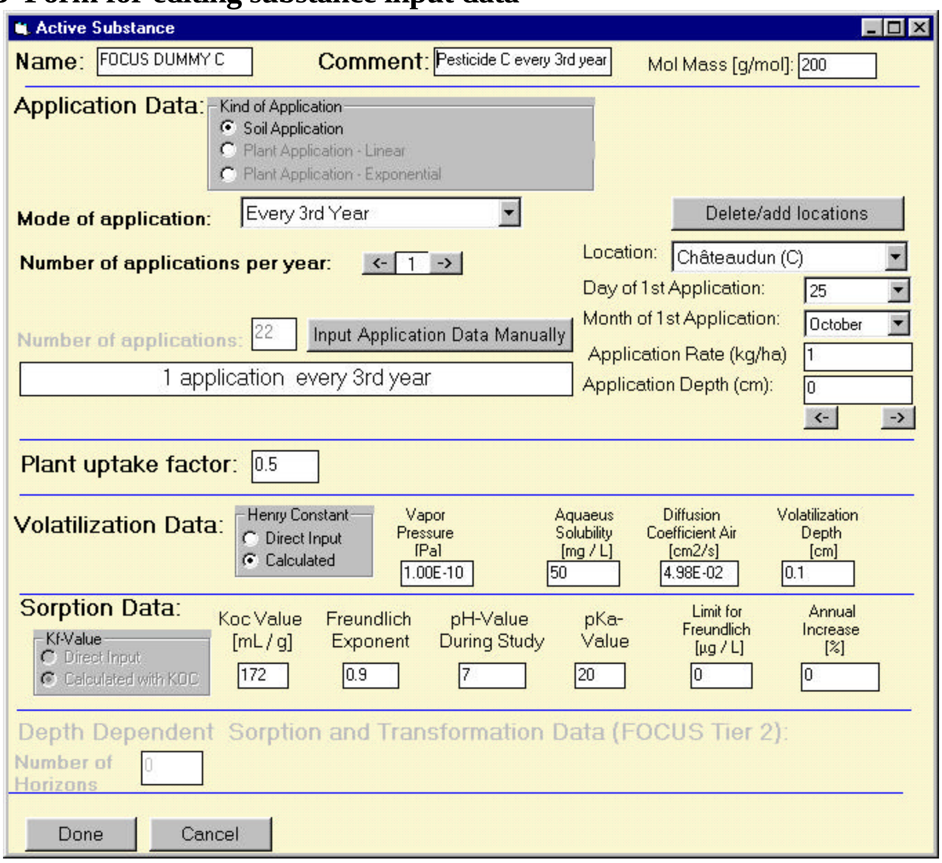
To create substance data files for PELMO using WPELMO the user has to follow two steps. First the metabolism scheme has to be defined (see Figure C.2)

Figure C.2 Edit the metabolism scheme



In the second step the user has to enter the necessary substance input data. There are specific forms for the substance (see Figure C.3) and for metabolites.

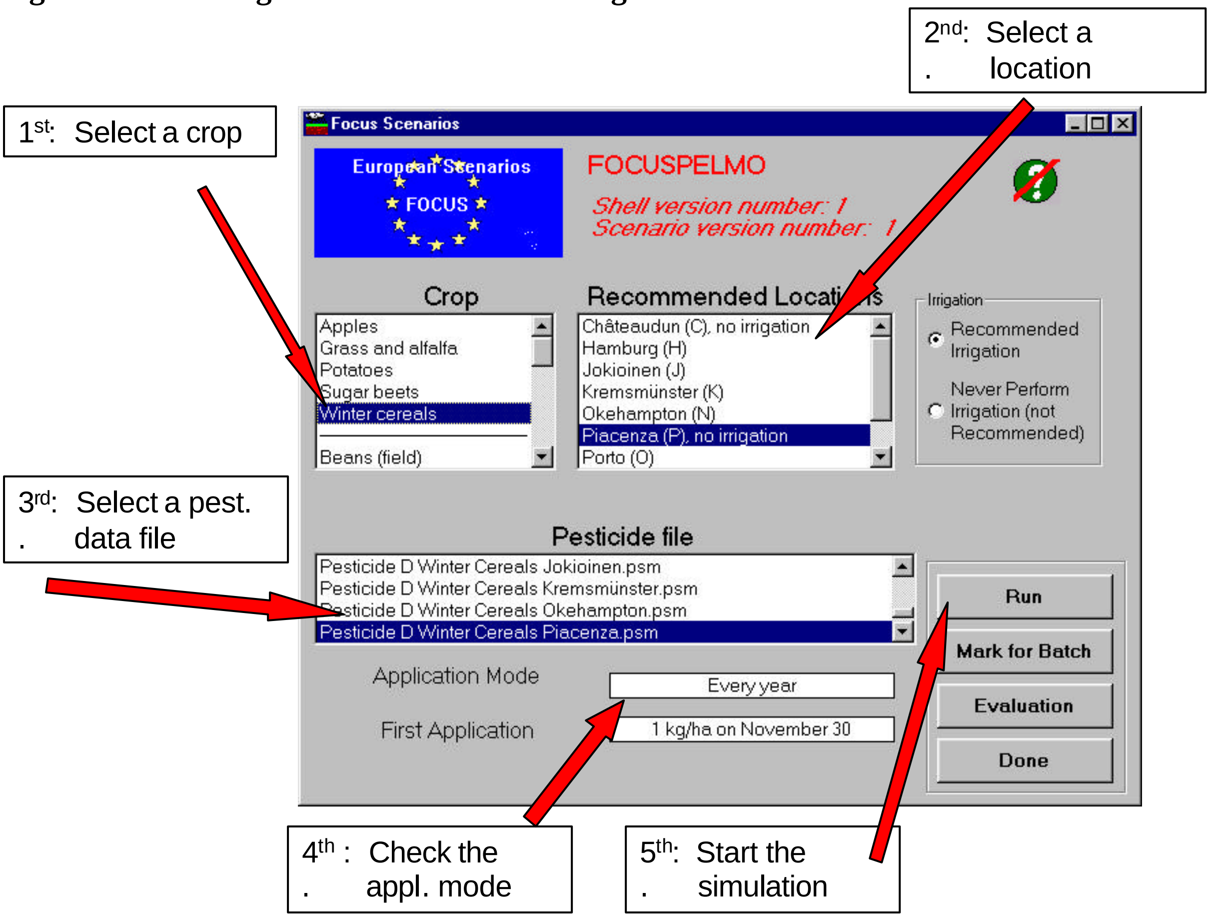
Figure C.3 Form for editing substance input data



Running simulations using WPELMO.EXE

Using the shell WPELMO.EXE it is easy to perform PELMO-simulations After having created a substance input data file (see Figure C.2 and Figure C.3) the user has to select a suitable crop and one of the recommended locations (see Figure C.4). The PELMO simulation will automatically start after clicking at the RUN button. It is not possible to run two PELMO simulations at the same time. Therefore, the RUN-button will be disabled as long as the current simulation is running.

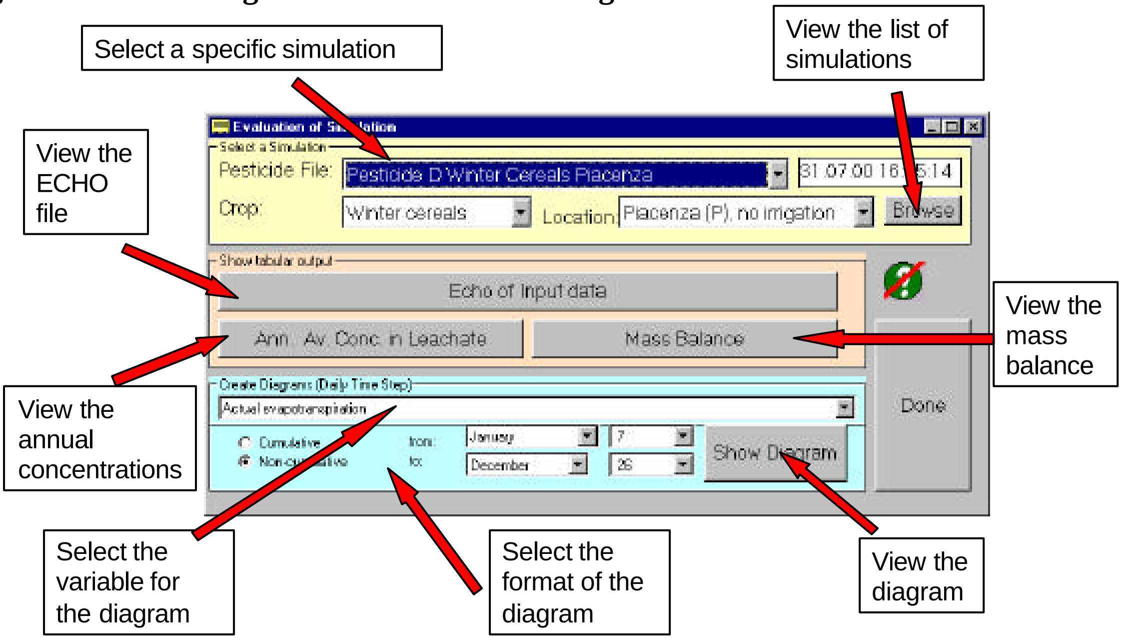
Figure C.4 Running PELMO simulations using WPELMO.EXE



Evaluating PELMO simulations using WPELMO.EXE

Using WPELMO it is easy to analyse all important results of a PELMO simulation. Specific modules of the shell generate annual average concentrations of substance and metabolites and calculate the 80th percentile. Additionally, time series diagrams of in total 23 parameters can be created with this shell. All variables can be visualised either in a cumulative or non-cumulative picture. The results of all evaluations can be transferred into other applications using the windows clipboard.

Figure C.5 Evaluating PELMO simulations using WPELMO.EXE



3 Parameterisation descriptions

The implemented scenario and parameter definitions are based on:

- **FOCUS DEFINITION** = Definitions made by the FOCUS working group
- **FOCUS SCENARIO SPECIFIC** = Definitions made by the FOCUS working group for a specific scenario
- **DEVELOPMENT DEFINITION** = Definitions made during the PELMO file development
- **USER INPUT** = Input to be specified by the user in the PELMO shell

Meteorological files (*.CLI)

Parameter and description	Value, source & comments
RECORD 1 TITLE: label for meteorological file	**FOCUS SCENARIO SPECIFIC**
RECORD 2 – REPEAT FOR EACH DAY OF A YR MMDDYY: meteorological month/day/year PRECIP: precipitation (cm day^{-1}) PEVP: pan evaporation data (cm day^{-1}) TEMP: 14h temperature per day (°C) AVTEMP: mean temperature per day (°C) VATEMP: difference between min. and max. temperature per day (°C) RELMOI: rel. humidity (%) – not used	**FOCUS SCENARIO SPECIFIC** Used are 9 location specific weather scenarios and 24 crop and location specific irrigated weather scenarios.

Soil scenario files (*.SZE)

Parameter and description		Value, source & comments
RECORD 1		
TITLE:	label for scenario title	**FOCUS SCENARIO SPECIFIC**
RECORD 2		
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 kc_year factors (see table with CN in record 9). These calibration factors reflect the soil surface and aerodynamic resistance as effective annual averages.
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 3.0
IPEIND:	pan factor flag	set to 0 = daily pan evaporation is read from the meteorological file - **FOCUS DEFINITION**
ANETD:	minimum depth of which evaporation is extracted (cm).	**DEVELOPMENT DEFINITION** - This location specific factor is highly correlated to the climatic conditions; based on the US distribution map and the relevant 20 year average annual air temperature following values are suggested for the specific FOCUS scenarios: (see table below) 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**
ISCOND:	surface condition of initial crop	set to 1 = fallow **DEVELOPMENT DEFINITION**

Scenario		Avg Temp	ANETD
CHÂTEAUDUN	C	11.3 °C	**20 cm**
HAMBURG	H	9.0 °C	**15 cm**
JOKIOINEN	J	4.1 °C	**10 cm**
KREMSMÜNSTER	K	8.6 °C	**15 cm**
OKEHAMPTON	N	10.2 °C	**15 cm**
PIACENZA	P	13.2 °C	**25 cm**
PORTO	O	14.8 °C	**25 cm**
SEVILLA	S	17.9 °C	**30 cm**
THIVA	T	16.2 °C	**30 cm**

RECORD 3 ERFLAG: flag to select simulation of erosion.	set to 0 = **no** erosion - **FOCUS DEFINITION**
RECORD 4 NDC: number of different crops in the simulation.	set to 1 = only **one** crop - **FOCUS DEFINITION**
RECORD 5 – REPEAT UP TO NDC ICNCN: crop number of the different crop.	set to 1 = the 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: 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 3.0, 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, bushberries citrus, grass, strawberries, vines) the same CN are used for fallow and residue!
USLEC:	Universal soil loss equation cover management factor for fallow, crop and residue.	Only required if ERFLAG = 1 set to 1 **– DEVELOPMENT DEFINITION**
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).
RECORD 6		
NCPDS:	number of cropping periods.	set to 66 (= longest possible simulation period) - **FOCUS DEFINITION**
RECORD 7 - REPEAT UP TO NCPDS		
E_MMDDYY:	crop emergence date (month/day/year).	**FOCUS SCENARIO SPECIFIC**
M_MMDDYY:	crop maturation date.	**FOCUS SCENARIO SPECIFIC**
H_MMDDYY:	crop harvest date.	**FOCUS SCENARIO SPECIFIC**
INCROP:	crop number associated with NDC	set to 1 (only one crop) - **FOCUS DEFINITION**
RECORD 8		
CORED:	total depth of soil core (cm)	**FOCUS SCENARIO SPECIFIC**
DUMMY:	dummy number	former plant uptake factor, not considered here any more, this parameter is now read in from the pesticide data file.
NCOM2	total number of simulation compartments in the soil core	**FOCUS SCENARIO SPECIFIC**
THFLAG:	field capacity and wilting point flag.	set to 0 = the **FOCUS SCENARIO SPECIFIC** soil water contents are used - **DEVELOPMENT DEFINITION** Comment: another PELMO option would be to calculate field capacity and wilting point by internal pedotransfer rules using scenario specific clay and sand contents.
HSWZT:	drainage flag.	set to 0 = free draining - **FOCUS DEFINITION**
RECORD 9		
NHORIZ:	total number of horizons	**FOCUS SCENARIO SPECIFIC**

RECORD 10A –REPEAT 10A-10B UP TO NHORIZ	
HORIZN: horizon number in relation to NRHORIZ.	**FOCUS SCENARIO SPECIFIC**
THKNS: soil horizon thickness (cm).	**FOCUS SCENARIO SPECIFIC**
BD: soil bulk density [g cm^{-3}]	**FOCUS SCENARIO SPECIFIC**
DISP: hydrodynamic dispersion (cm^2 day^{-1})	set to 0, dispersion is accounted for in PELMO by numerical dispersion – **FOCUS DEFINITION**
THETO: initial soil water content in the soil horizon (cm^3 cm^{-3})	set to 0.2 – **DEVELOPMENT DEFINITION**
RECORD 10B –REPEAT 10A-10B UP TO NHORIZ	
THEFC: field capacity (cm^3 cm^{-3}).	**FOCUS SCENARIO SPECIFIC**
THEWP: wilting point (cm^3 cm^{-3}).	**FOCUS SCENARIO SPECIFIC**
OC: organic carbon content (%)	**FOCUS SCENARIO SPECIFIC**
PH: pH value	**FOCUS SCENARIO SPECIFIC**
Biodeg: relative biodegradation factor	depth dependent correction factor applied to the substance(s) degradation rates **FOCUS DEFINITION** 0 – 30 cm depth 1 30 – 60 cm depth 0.5 60 – 100 cm depth 0.3 > 100 cm depth 0
RECORD 11	
ILP: Initial level of substance indicator	set to 0 = no initial substance levels input – **DEVELOPMENT DEFINITION**
RECORD 12	
ITEM1: Hydrology output summary indicator	**DEVELOPMENT DEFINITION**
STEP1: Time step of hydrology output	set to YEARLY – **DEVELOPMENT DEFINITION**
LFREQ1: Frequency of soil compartment reporting	set to 1 = every compartment is output –**DEVELOPMENT DEFINITION**
ITEM2: Substance output summary indicator	**DEVELOPMENT DEFINITION**
STEP2: Time step of substance output	set to YEARLY – **DEVELOPMENT DEFINITION**
LFREQ2: Frequency of soil compartment reporting	set to 1 = every compartment is output –**DEVELOPMENT DEFINITION**
ITEM3: Substance concentration profile indicator	**DEVELOPMENT DEFINITION**
STEP3: Time step of substance concentration profile output	set to YEARLY – **DEVELOPMENT DEFINITION**
LFREQ3: Frequency of soil compartment reporting	set to 1 = every compartment is output –**DEVELOPMENT DEFINITION**

RECORD 13 NPLOTS: Number of time series to be written to plotting file	22 **- DEVELOPMENT DEFINITION**
RECORD 14 – REPEAT UP TO NPLTOTS PLNAME: Identifier of time series MODE: Plotting mode IARG: Argument of variable identified in PLNAME CONST: Constant used for unit conversion	**DEVELOPMENT DEFINITION** Comment: The time series identified here are requirements for the graphical output and analysis within the Graphical User Interface. They cannot be changed.
RECORD 15 ROFLAG: Runoff flag DEPRO: infiltration depth before runoff starts (cm)	set to 1 = runoff calculated – **FOCUS DEFINITION** set to 5.0 cm – **DEVELOPMENT DEFINITION**
RECORD 16 GEOBREI: Latitude	**FOCUS SCENARIO SPECIFIC** Comment: The geographical latitude is usually required only for calculation of the evapotranspiration by the methods of Hamon or Haude, whereas the **FOCUS DEFINITION** is to use daily pan evaporation data.

Substance file (*.PSM)

Parameter and description	Value, source & comments
Comment: Text and / or lines in the substance file that are given in brackets (< >) are comments for easier understanding of the file structure and mark the beginning or end of a parameter section. These lines should not be changed. The compound parameters are described here only for the parent compound. In principle, all processes except from volatilisation are taken into account also for each metabolite. Therefore, for each metabolite to be simulated, a similar set of parameters needs to be included, leaving out only the volatilisation data.	
COMMENT CTITLE: label for substance	**USER INPUT**
SOIL HORIZONS NHORIZ: total number of soil horizons	set to 0 = not used - **DEVELOPMENT DEFINITION** Comment: This parameter is required if depth dependent biodegradation factors are specified in the substance file instead of the scenario file. The parameter has then to be set to the scenario specific number of horizons.
NUMBER OF LOCATIONS N_LOC: number of locations for which applications will be defined (1-10)	**FOCUS SCENARIO SPECIFIC / USER INPUT**

APPLICATIONS - REPEAT UP TO N_LOC NAPS: total number of substance applications occurring at different dates (1 – 200).	**FOCUS SCENARIO SPECIFIC / USER INPUT**
APPLICATIONS – REPEAT UP TO NAPS	
APD: Day of the month of application	**USER INPUT**
APM: Month of application	**USER INPUT**
IAPYR: Year of application	**USER INPUT**
TAPP: Total application rate (kg ha^{-1})	**USER INPUT**
DEPI: Depth of incorporation (cm)	**USER INPUT**
APPLICATION MODE FAM: Substance application model	**USER INPUT** Selectable chemical application methods are: **1** = application to soil only **2** = foliar application using the linear model **3** = non-linear foliar application using exponential filtration model **Note:** Foliar application needs to be activated to simulate washoff from plant foliage and degradation of foliage substance.
FOLIAR APPLICATION PARAMETERS (ONLY IF FAM = 2 OR 3)	
PLDKRT: Decay rate on the plant foliate ($days^{-1}$)	Not used for FOCUS scenarios
FEXTRC: Foliar extraction coefficient for substance washoff per cm of precipitation	Not used for FOCUS scenarios
FILTRA: Filtration parameter. Only required for exponential model (FAM = 3).	Not used for FOCUS scenarios
FLAGS	
VAPFLG: Henry's constant flag	**USER INPUT** **0** = Henry's constant input by user **1** = Henry's constant calculated
KDFLAG: K_D flag	**USER INPUT** **0** = K_D input by user **1** = K_D calculated from K_{OC}

VOLATILISATION		
HENRYK:	normalised Henry's law constant of the active substance (dimensionless).	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)
SOLUB:	Solubility in water (mg L^{-1})	**USER INPUT**
MOLMAS:	Molar mass (g mol^{-1})	**USER INPUT**
VAPPRE:	Vapour pressure (Pa)	required for calculation of Henry's constant - **USER INPUT**
DAIR:	molecular diffusion coefficient for the substance(s) in the air (cm^2 sec^{-1})	required for calculation of Henry's constant - **USER INPUT**
VOLGRE:	depth for volatilisation (cm)	set to 0.1 cm – **FOCUS DEFINITION**
PLANT UPTAKE		
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!
DEGRADATION - REPEAT FOR METABOLISATION PATHS A1 – D1 AND BOUND RESIDUES / CO_2		
DKRATE:	degradation rate constant (day^{-1})	**USER INPUT -** Can also be entered as a DT50 value
TEMP0:	reference temperature for the degradation rate constant (°C)	**USER INPUT**
Q10:	Q10-factor for degradation rate increase when temperature increases by 10°C	**USER INPUT** default = 2.2 - **FOCUS DEFINITION**
ABSFEU:	absolute reference moisture content during the degradation studies (%Vol)	**USER INPUT**
FELFEU:	relative reference moisture content during the degradation studies (% of FC (field capacity))	**USER INPUT** Comment: either absolute or relative soil moisture has to be specified, the other parameter should be set to 0
FEUEXP:	Exponent for the moisture dependent correction of the degradation rate constant (moisture relationship according to WALKER)	**USER INPUT** default = 0.7 – **FOCUS DEFINITION**

ADSORPTION (IF KDFLAG = 1)		
KOC:	K_{OC} value (ml g^{-1})	**USER INPUT**
FRNEXKOC:	Freundlich exponent 1/n (dimensionless)	**USER INPUT**
PH_KOC:	pH value	**USER INPUT** default = 7
PKA:	pKA value	**USER INPUT** default = 20, ie in practice not used
FRNMIN:	lower limit concentration for the non-linear sorption according to Freundlich (µg L^{-1})	**USER INPUT** default = 0.01 µg L^{-1}
ALTERN:	annual increase of adsorption (%)	**USER INPUT** default = 0 (no increase of sorption with time)
DEPTH DEPENDENT SORPTION (IF KDFLAG = 0) – REPEAT FOR EACH SOIL HORIZON		
KD :	K_D value (ml g^{-1})	**USER INPUT**
FRNEXP:	Freundlich exponent 1/n (dimensionless)	**USER INPUT**
DEG(1):	depth dependent correction of degradation rate for metabolism path A1	**USER INPUT**
DEG(2):	depth dependent correction of degradation rate for metabolism path B1	**USER INPUT**
DEG(3):	depth dependent correction of degradation rate for metabolism path C1	**USER INPUT**
DEG(4):	depth dependent correction of degradation rate for metabolism path D1	**USER INPUT**
DEG(5):	depth dependent correction of degradation rate for metabolism path BR/CO2	**USER INPUT**
		Comment: the depth dependent correction of degradation can also be specified in the scenario file. According to **FOCUS DEFINITION** the depth dependent correction factors are 0 – 30 cm depth 1 30 – 60 cm depth 0.5 60 – 100 cm depth 0.3 > 100 cm depth 0

Control file PELMO.INP

Parameter and description		Value, source & comments
RECORD 1		
IYEAR:	number of years of simulation period	26, 46, or 66 years - **FOCUS DEFINITION**
ISDAY:	start day of simulation	1 – **DEVELOPMENT DEFINITION**
ISMON:	start month of simulation	1 - **DEVELOPMENT DEFINITION**
IEDAY:	end day of simulation	31 - **DEVELOPMENT DEFINITION**
IEMON:	end month of simulation	12 - **DEVELOPMENT DEFINITION**
RECORD 2		
APPLIK:	scenario parameter file name	**USER INPUT, FOCUS DEFINITION**
RECORD 3		
CHEM:	substance parameter file name	**USER INPUT**
RECORD 4 - REPEAT UP TO (NUMBER OF SIMULATION YEARS)		
KLIMA:	climate file name	**USER INPUT, FOCUS DEFINITION**

4 References

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Dean, J. D., P. S. Huyakorn, A. S. Donigian, K. A. Voos, R. W. Schanz, Y. J. Meeks, and R. F. Carsel. 1989a. Risk of Unsaturated/Saturated Transport and Transformation of Chemical Concentrations (RUSTIC). Volume 1: Theory and Code Verification, EPA/600/3-89/048a. U. S. EPA Environmental Research Laboratory, Athens, GA.

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OECD (1997): Approved draft proposal for an updated OECD guidance document No. 106: Adsorption/Desorption. OECD Guidelines for Testing of Chemicals, 1-44.

APPENDIX D . PARAMETERISATION OF PRZM

1 Introduction

A modified and improved PRZM code (version 3.2, 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 32bit FORTRAN compiler. The new PRZM31 executable WINPRZM.EXE is now independent from any DOS limitations. 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 PRZM31 code (Version 3.2, FOCUS release).

The information necessary to run PRZM31.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.

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, as required for FOCUS.

2 Parameter description

PARAMETER AND DESCRIPTION	VALUE, SOURCE & COMMENTS
Meteorological files MMDDYY: meteorological month/day/year 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)	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**
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 kc_year factors, (see table with CN in record 9). These calibration factors reflect the soil surface and aerodynamic resistance as effective annual averages.
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 0 = daily pan evaporation is read from the meteorological file - **FOCUS DEFINITION**
ANETD: minimum depth of which evaporation is extracted (cm).	**DEVELOPMENT DEFINITION** - This location specific factor is highly correlated to the climatic conditions; based on the US distribution map and the relevant 20 year average annual air temperature following values are suggested for the specific FOCUS scenarios: CHÂTEAUDUN C 11.3 °C **20 cm** HAMBURG H 9.0 **15 cm** JOKIOINEN J 4.1 **10 cm** KREMSMÜNSTER K 8.6 **15 cm** OKEHAMPTON N 10.2 **15 cm** PIACENZA P 13.2 **25 cm** PORTO O 14.8 **25 cm** SEVILLA S 17.9 **30 cm** THIVA T 16.2 **30 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**

ISCOND: surface condition of initial crop DSN: WDM data set (5 numbers)	set to 1 = fallow - **DEVELOPMENT DEFINITION** not used in the input files - **DEVELOPMENT DEFINITION**
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: 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, bushberries 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 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).	**FOCUS SCENARIO SPECIFIC**
M_DDMMYY: crop maturation date.	**FOCUS SCENARIO SPECIFIC**
H_DDMMYY: crop harvest date.	**FOCUS SCENARIO SPECIFIC**
INCROP: crop number associated with NDC	set to 1 (only one crop) - **FOCUS DEFINITION**
Record 13 NAPS: total number of substance applications occurring at different dates (1 to 50).	**FOCUS SCENARIO SPECIFIC / USER INPUT** (User can specify in the PRZM shell up to 10 annual substance applications.)
NCHEM: number of substance(s) in the simulation.	**USER INPUT** set to 1 = parent only set to 2 = parent with metabolite set to 3 = parent with two metabolites
FRMFLG: flag for testing of ideal soil moisture conditions for the application of substance relative to the target date.	set to 0 = **no** moisture test - **FOCUS DEFINITION**
DKFLG2 flag to allow input of bi-phase half-life.	**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 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** for use with

	FOCUS scenarios. **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) should be used for TIER 1 modelling of applications made to the soil surface. Actual runoff results and experience from Waterborne suggest that this PRZM default is much more appropriate to simulate 'realistic' runoff than a thin-layer soil surface application! By doing so the soil surface roughness is also considered in an realistic way. Test runs have shown, that the leaching concentrations below 1 m depth are not significantly affected.
TAPP: target application rate (kg ha^{-1}).	**USER INPUT**
APPEFF: application efficiency (fraction).	**USER INPUT** default = set to 1 (no application loss) Default value not to be changed for TIER 1 modelling!
DRFT: spray drift (fraction).	**USER INPUT** default = set to 0 (no spray drift) Default value not to be changed for TIER 1 modelling!
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 modeling since crop interception to be set to zero.
PLDKRT: substance decay rate on plant foliage ($days^{-1}$).	**USER INPUT** Not relevant for TIER 1 modeling since crop interception to be

FEXTRC: foliar extraction coefficient for substance washoff per centimetre of rainfall	set to zero. **USER INPUT** Not relevant for TIER 1 modeling 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. BDFLAG: bulk density flag. THFLAG: field capacity and wilting point flag. KDFLAG: flag to select soil/substance adsorption coefficient (KD, Koc or normalised Freundlich using C_{ref} = 1 mg L^{-}, aged sorption KD_{aged}). HSWZT: drainage flag. MOC: method of characteristics flag. IRFLAG: irrigation flag.	**FOCUS SCENARIO SPECIFIC** set to 0 = soil specific bulk density is used - **DEVELOPMENT DEFINITION** set to 0 = the **FOCUS SCENARIO SPECIFIC** soil water contents are used - **DEVELOPMENT DEFINITION** <u>Comment:</u> another PRZM option would be to calculate field capacity and wilting point by using scenario specific clay and sand contents. **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**. set to 0 = free draining - **FOCUS DEFINITION** set to 0 = not used - **DEVELOPMENT DEFINITION** <u>Comment:</u> 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. 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) IDFLAG: flag to select thermal conductivity and heat capacity BIOFLAG: biodegradation flag	**FOCUS SCENARIO SPECIFIC** <u>Comment:</u> 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)! set to 1 = PRZM simulates automatically soil temperature profiles without the need of thermal conductivity and heat capacity - **DEVELOPMENT DEFINITION** <u>Comment:</u> Thermal conductivity and heat capacity data is not specified in the FOCUS data. set to 0 = special multiphase biodegradation using a detailed definition of micro-organism populations is **not** used - **FOCUS DEFINITION**
Record 26 DAIR: molecular diffusion coefficient for the substance(s) in the air. (**cm^2 day^{-1}**) HENRYK: normalised Henry's law constant of the substance(s). (dimensionless) ENPY: enthalpy of vaporisation of the substance(s). (kcal $mole^{-1}$)	set to 4300 = **FOCUS DEFINITION** (0.43 $m^2 day^{-1}$ = 4300 $cm^2 day^{-1}$) set to a value calculated from the PRZM shell depending on other **USER INPUT** <u>Comment:</u> 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) set to 22.7 kcal $mole^{-1}$ - **FOCUS DEFINITION**
Record 30 (only if KDFLAG = 1) PCMC: flag to select which model is used to estimate KD (see record 37). SOL: substance(s) Koc entered according to PCMC flag above for each NCHEM.	set to 4 = Koc in L kg^{-1} depending on **USER INPUT** **USER INPUT**
Record 30b (only if KDFLAG = 2 or 3) FRNDCF: 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 0.01 µg L^{-1}.	**USER INPUT** Normalised Freundlich is implemented in PRZM in the same way as in PELMO and in PEARL. - **DEVELOPMENT DEFINITION** **NOTE:** 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.
Record 30c (only if KDFLAG = 3) BAKD: Time points for the definition of the ageing factors VAKD (days) - 5 values VADK: Time dependent factor (5 dimensionless values) to calculate an aged sorption:	**USER INPUT** default = not used - **FOCUS DEFINITION** Aged sorption is not to be used in the FOCUS scenarios unless experimental data is available.

KD_{aged} = VADK * KD	Comment: Aged sorption is described with an dimensionless time dependent ageing factor > 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 neighboring 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 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: Q10-factor for degradation rate increase when temperature increases by 10°C TBASE: temperature during the test of biodegradation	**USER INPUT** default = 2.2 - **FOCUS DEFINITION** **USER INPUT**
Record 32b (only if ITFLAG = 2) absrel: flag to select if reference soil moisture for moisture corrected degradation is given absolute or relative to FC (field capacity) B-value: exponent of moisture corrected degradation (moisture relationship according to WALKER) refmoist: reference soil moisture	**USER INPUT** (absolut: absrel = 1; relative to FC: absrel = 2) **USER INPUT** default = 0.7 - **FOCUS DEFINITION** **USER INPUT**
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. THKNS: thickness of the horizon. BD: bulk density (kg/L). THETO: initial soil water content in the horizon (cm^3 cm^{-3}). AD: soil drainage parameter (day^{-1}). (only required if HSWZT = 1) DISP: substance(s) hydrodynamic solute dispersion/diffusion coefficient. (cm^2 day^{-1}) ADL: lateral soil drainage parameter (day^{-2}). (only required if HSWZT = 1).	**FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC** set to field capacity from FOCUS soil data - **DEVELOPMENT DEFINITION** set to 0 = not used - **FOCUS DEFINITION** set to 0 - **DEVELOPMENT DEFINITION** (DISP is only used for MACRO and PEARL) set to 0 = not used - **FOCUS DEFINITION**
Record 36 (for DKFLG2 = 0) DWRATi: dissolved phase substance(s) decay rate for first phase (day^{-1}). DSRATi: adsorbed phase substance(s) decay rate for first phase (day^{-1}). DGRATi: vapour phase substance(s) decay rate for first phase (day^{-1}).	Based on a lumped degradation the two parameters DWRATi and DSRATi are set from the shell for each compound (index I for parent and metabolites) to the substance degradation rate specified by the **USER INPUT.** - **DEVELOPMENT DEFINITION** 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) DWRAT2i: dissolved phase pesticide(s) decay rate for second phase of bi-phase reaction (day^{-1}). DSRAT2i: adsorbed phase pesticide(s) decay rate for second phase of bi-phase reaction (day^{-1}). DGRAT2i: vapour 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 set to 0 - DEVELOPMENT DEFINITION
Record 37 DPN: thickness of compartments in the horizon (cm). THEFC: field capacity in the horizon (cm^3 cm^{-3}). THEWP: wilting point in the horizon (cm^3 cm^{-3}). OC: organic carbon in the horizon (percent). KD: layer specific substance(s) partition coefficient for each NCHEM. (L kg^{-1}).	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 volatilization viewpoint, a smaller DPN in the top horizon is required for better estimation of the volatilization 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 volatilization is a major loss mechanism (PRZM default, see PRZM 3.12 manual). **FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC** **FOCUS SCENARIO SPECIFIC / USER INPUT** (required if KDFLAG = 0 or 2, else set to 0.0)
Record 38 (only if ITFLAG = 1 or 2) SPT: initial temp. of the horizon (Celsius). SAND: sand content in the horizon (percent). CLAY: clay content in the horizon (percent). THCOND: thermal conductivity of the horizon (cm^{-1} day^{-1}). VHTCAP: heat capacity per unit volume of the soil horizon (cm^{-3} $Celsius^{-1}$).	calculated bottom temperatures - **DEVELOPMENT DEFINITION** SAND and CLAY contents are set to 0 - values only required if THFLAG = 1 - **DEVELOPMENT DEFINITION** set to 0 - only required if IDFLAG = 0 - **DEVELOPMENT DEFINITION** 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**

3 References

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