

TEXTE

201/2020

Evaluation of the risk for soil organisms under real conditions

Development of a national position for amending
downstream legislations of the new EU Plant Protection
Products Regulation

Appendix

TEXTE 201/2020

Environmental Research of the
Federal Ministry for the
Environment, Nature Conservation
and Nuclear Safety

Project No. (FKZ) 3710 67 410
Report No. EF001129-ANH,ENG

Evaluation of the risk for soil organisms under real conditions

Development of a national position for amending downstream legislations of the
new EU Plant Protection Products Regulation

Appendix

by

Andreas Toschki (Coordination), Monika Hammers-Wirtz
gaiaac -Research Institute for Ecosystem Analysis and Assessment, Aachen

Claudia Poßberg, Martina Roß-Nickoll, Andreas Schäffer, Burkhard Schmidt,
Björn Scholz Starke
RWTH Aachen University, Aachen

Jörg Römbke, Adam Scheffzyk
ECT- Oekotoxikologie GmbH, Flörsheim am Main

Michael Klein, Udo Hommen
Fraunhofer IME, Schmallenberg

On behalf of the German Environment Agency

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 /umweltbundesamt.de

 /umweltbundesamt

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gaiaac-Research Institute for Ecosystem Analysis and Assessment e.V.
Kackertstr. 10
52072 Aachen

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1 Appendix: Prescreening and soil characterization- soil analysis of external company



Lochhausener Str. 205
81249 München
Telefon +49(0)89/ 863 005-0
Telefax +49(0)89/ 863 005-11
e-Mail: info@labor-graner.de
internet: www.labor-graner.de

Dr. Graner & Partner GmbH, Lochhausener Str. 205, 81249 München

München, 09.06.2011

Forschungsinstitut gaiac – c/o:
RWTH Aachen, Inst. f. Umweltforschung
Worringerweg 1

52056 Aachen

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Projektleiter: Herr Dr. Toschki
Auftrags-Nr.:
Auftraggeberprojekt: Bodenproben Eifelwiese
Probenahmedatum: 04.04.2011
Probenahmeort:
Probenahme durch: Auftraggeber
Probengefäße: Kunststoff - Beutel
Eingang am: 07.04.2011
Beginn/Ende Prüfung: 07.04.2011 – 18.05.2011

Die Prüfergebnisse beziehen sich ausschließlich auf den Prüfgegenstand. Eine auszugsweise Vervielfältigung des Prüfberichtes ist nur mit schriftlicher Genehmigung der Prüflaborleitung erlaubt. Die in den zitierten Normen und Richtlinien angegebenen Meßunsicherheiten werden eingehalten. Unsachgemäße Probengefäße können zu Verfälschungen des Messwertes führen. Prüfergebnisse von Mischproben die unterhalb des Grenzwertes liegen, können trotzdem zu Grenzwertüberschreitungen von einer oder mehreren Teilproben führen. Um die Überprüfung des Grenzwertes sicher zu gewährleisten, wird angeraten, gemäß Prüfvorschrift die Einzelproben zu untersuchen. Mikrobiologisches Untersuchungsmaterial wird nach der Auswertung sofort vernichtet.

Akkreditiertes Prüflabor nach DIN EN ISO 17025 · DAR-Reg.-Nr.: DAP-PA-2295.01

Arzneimittel, Lebensmittel, Kosmetika, Bedarfsgegenstände, Wasser, Boden, Luft, Medizinprodukte
Analytik, Entwicklung, Qualitätskontrolle, Beratung, Sachverständigengutachten, amtliche Gegenproben, Mikrobiologie, Arzneimittelzulassung,
Abgrenzungsfragen AMG/LMBG

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BIC: GENODEF333, IBAN: DE30 7016 9484 0000 0699 22

Prüfbericht: 1106099 09.06.2011
 Auftraggeberprojekt: Bodenproben Eifelwiese

Probenbezeichnung: Höf / INT 0-5 cm Oberboden

Probenahmedatum: 04.04.2011

Labornummer: 1106099-001

Material: Feststoff

	Gehalt	Einheit	BG	Methode
Trockenrückstand	69	%		ISO 11465
Kationenaustauschkapazität	56	mmol/kg TS	0,1	DIN ISO 11260
Gesamtstickstoff	5700	mg/kg TS	10	DIN 38409 - H12
Phosphor	1600	mg/kg TS	5	EN ISO 11885 (E22)
Atrazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Desethylatrazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Sebuthylazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Simazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Terbutylazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Hexazinon	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Chlortoluron	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Diuron	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Isoproturon	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Methabenzthiazuron	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Metobromuron	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Metazachlor	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Mecoprop	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
MCPA	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Dichlorprop (2,4-DP)	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Bentazon	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Monuron	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Carbofuran	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Desisopropylatrazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Propazin	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Bromacil	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Parathion-ethyl	u.d.B.	mg/kg TS	0,01	EN ISO 11369 (F12)/ HPLC-MS/MS
Lindan	u.d.B.	mg/kg TS	0,01	DIN 38407 - F2/ GC-MS
Heptachlor	u.d.B.	mg/kg TS	0,01	DIN 38407 - F2/ GC-MS
Heptachlorepoxyd	u.d.B.	mg/kg TS	0,01	DIN 38407 - F2/ GC-MS
Aldrin	u.d.B.	mg/kg TS	0,01	DIN 38407 - F2/ GC-MS
Dieldrin	u.d.B.	mg/kg TS	0,01	DIN 38407 - F2/ GC-MS
Summe PSM nach TrinkwV	0	mg/kg TS		berechnet

Dr. Graner & Partner GmbH
 Labor für analytische und pharmazeutische Chemie
 Sachverständigenbüro

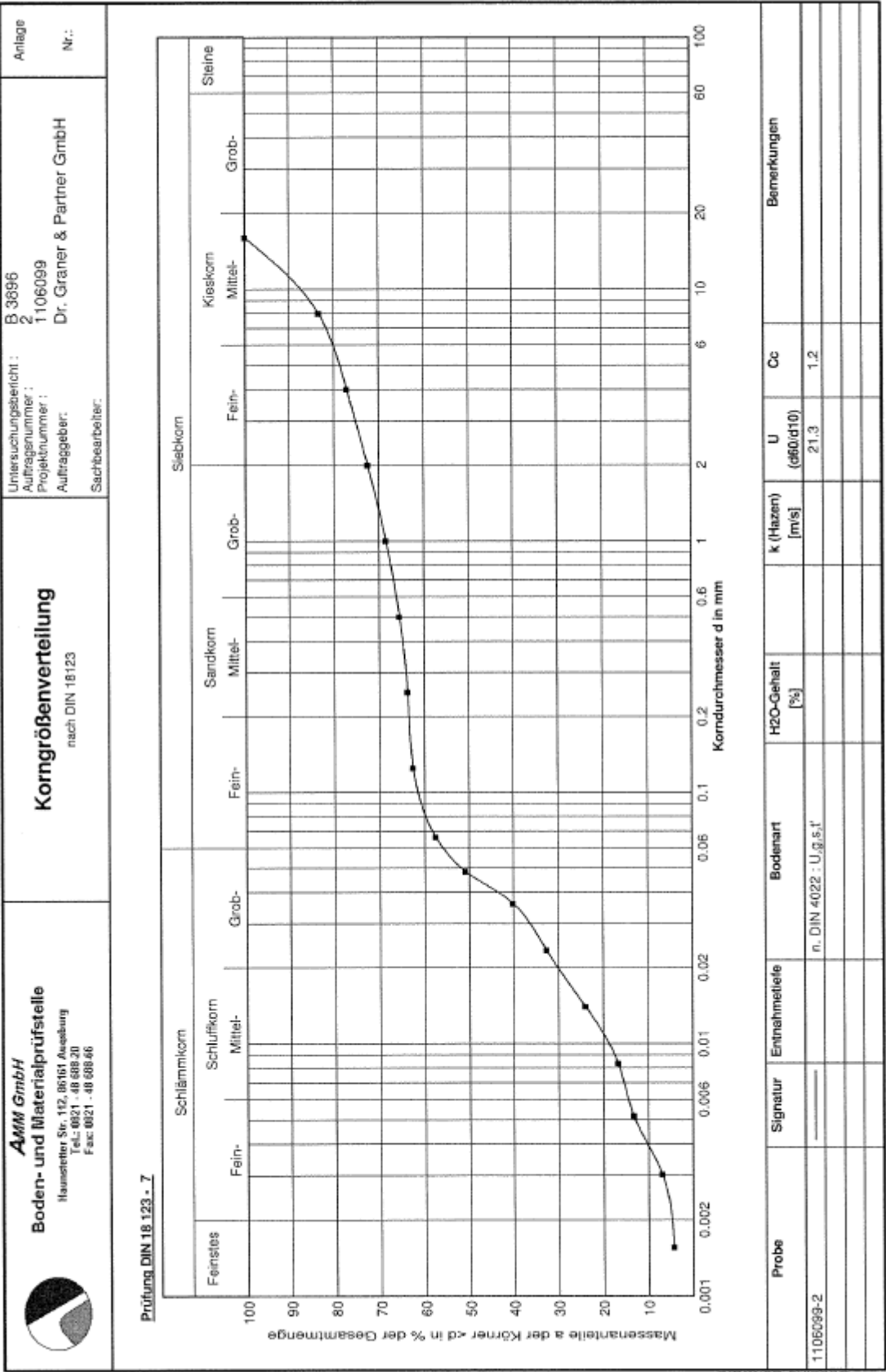
Prüfbericht: 1106099 09.06.2011
 Auftraggeberprojekt: Bodenproben Eifelwiese

Probenbezeichnung:	Höf / INT 0-5 cm Oberboden			
Probenahmedatum:	04.04.2011			
Labornummer:	1106099-002			
Material:	Feststoff			
	Gehalt	Einheit	BG	Methode
pH-Wert	6,5			DIN ISO 11265
Trockenrückstand	69	%		ISO 11465
TOC	4,7	% TS	0,1	DIN EN 13137

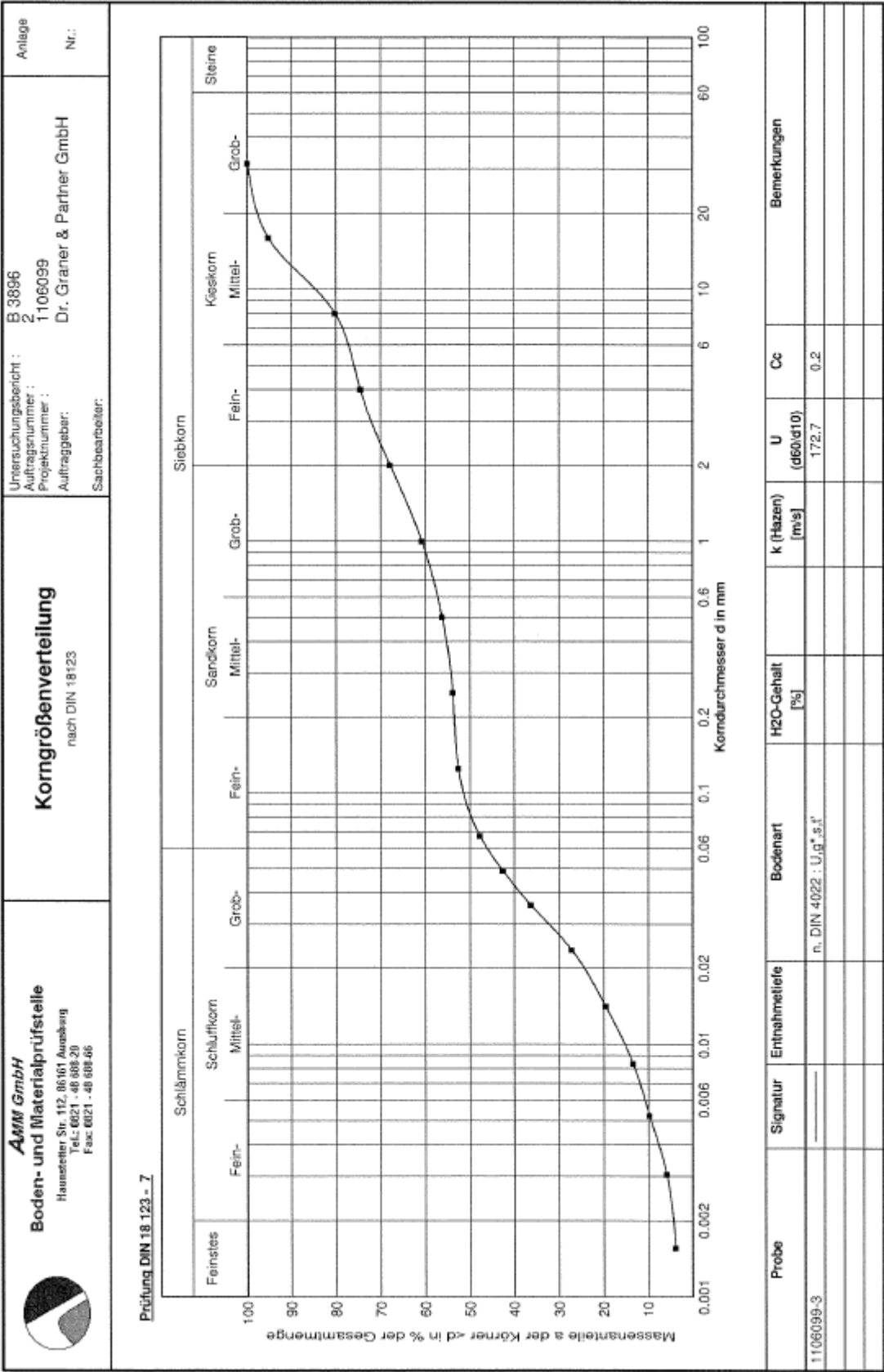
Probenbezeichnung:	Höf / INT 5-10 cm			
Probenahmedatum:	04.04.2011			
Labornummer:	1106099-003			
Material:	Feststoff			
	Gehalt	Einheit	BG	Methode
pH-Wert	6,1			DIN ISO 11265
Trockenrückstand	76	%		ISO 11465
TOC	3,1	% TS	0,1	DIN EN 13137

Probenbezeichnung:	Höf / INT 15-25 cm			
Probenahmedatum:	04.04.2011			
Labornummer:	1106099-004			
Material:	Feststoff			
	Gehalt	Einheit	BG	Methode
pH-Wert	6,2			DIN ISO 11265
Trockenrückstand	78	%		ISO 11465
TOC	2,7	% TS	0,1	DIN EN 13137

BG = Bestimmungsgrenze
 u.d.B. = unter der Bestimmungsgrenze



 AMM GmbH Boden- und Materialprüfstelle Haunstetter Str. 112, 86161 Augsburg Tel.: 0821 - 48 688 20 Fax: 0821 - 48 688 66	Korngrößenverteilung nach DIN 18123	Anlage Nr.:																																																																																																																								
Untersuchungsbericht : B 3896 Auftragsnummer : 2 Projektnummer : 1106099 Auftraggeber: Dr. Graner & Partner GmbH Probe : 1106099-2 Bodenart : n. DIN 4022 : U,g,s,l' Ort : Tiefe : Probengefäß : Braunglas Datum : Person : Witterung :																																																																																																																										
Siebanalyse <table border="1" style="width: 100%; border-collapse: collapse; text-align: center;"> <thead> <tr> <th rowspan="2">Korngröße [mm]</th> <th colspan="2">Rückstände</th> <th rowspan="2">Summe Sieb- durchgänge [%]</th> </tr> <tr> <th>Masse [g]</th> <th>Anteil [%]</th> </tr> </thead> <tbody> <tr><td>90.0</td><td></td><td></td><td></td></tr> <tr><td>63.0</td><td></td><td></td><td></td></tr> <tr><td>31.5</td><td></td><td></td><td></td></tr> <tr><td>16.0</td><td></td><td></td><td>100.0</td></tr> <tr><td>8.0</td><td>26.4</td><td>16.6</td><td>83.4</td></tr> <tr><td>4.0</td><td>10.0</td><td>6.3</td><td>77.1</td></tr> <tr><td>2.0</td><td>7.2</td><td>4.5</td><td>72.6</td></tr> <tr><td>1.0</td><td>6.6</td><td>4.2</td><td>68.4</td></tr> <tr><td>0.5</td><td>4.6</td><td>2.9</td><td>65.5</td></tr> <tr><td>0.250</td><td>2.9</td><td>1.8</td><td>63.7</td></tr> <tr><td>0.125</td><td>1.8</td><td>1.1</td><td>62.6</td></tr> <tr><td>0.063</td><td></td><td></td><td></td></tr> <tr><td>Schale</td><td>99.4</td><td>62.6</td><td></td></tr> <tr><td>Summe</td><td>158.9</td><td>100.0</td><td></td></tr> <tr><td>Siebverlust</td><td></td><td></td><td></td></tr> </tbody> </table> Prüfung DIN 18 123 - 7 <u>allgemeine Angaben zur Siebanalyse</u> Datum : 12.04.2011 Person : Marz Trockenmasse [g] : 158.9 Größtkorn [mm] : Kornform : <u>allgemeine Angaben zur Sedimentation</u> Datum : 18.05.2011 Person : Schuster Trockenmasse [g] : 34.6 Korndichte [g/cm³] : 2.680 Ärömeter : 8873 Dispergierungsmittel : Natriumpyrophosphat Meniskuskorrektur : 1.10 100% Lesung : 21.7 Hilfswert : 4.61			Korngröße [mm]	Rückstände		Summe Sieb- durchgänge [%]	Masse [g]	Anteil [%]	90.0				63.0				31.5				16.0			100.0	8.0	26.4	16.6	83.4	4.0	10.0	6.3	77.1	2.0	7.2	4.5	72.6	1.0	6.6	4.2	68.4	0.5	4.6	2.9	65.5	0.250	2.9	1.8	63.7	0.125	1.8	1.1	62.6	0.063				Schale	99.4	62.6		Summe	158.9	100.0		Siebverlust																																																									
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 AMM GmbH Boden- und Materialprüfstelle Haunsteiner Str. 112, 86161 Augsburg Tel.: 0821 - 40 688-20 Fax: 0821 - 40 688-66	Korngrößenverteilung nach DIN 18123	Anlage Nr.:
Untersuchungsbericht : B 3896 Auftragsnummer : 2 Projektnummer : 1106099 Auftraggeber: Dr. Graner & Partner GmbH Probe : 1106099-3 Bodenart : n. DIN 4022 : U,g*,s,t		
Ort : Tiefe : Probengefäß : Braunglas Datum : Person : Witterung :		

Siebanalyse

Korngröße [mm]	Rückstände		Summe Sieb- durchgänge [%]
	Masse [g]	Anteil [%]	
90.0			
63.0			
31.5			100.0
16.0	8.8	4.7	95.3
8.0	28.0	15.1	80.2
4.0	10.3	5.5	74.7
2.0	12.5	6.7	67.9
1.0	13.4	7.2	60.7
0.5	8.3	4.5	56.2
0.250	4.5	2.4	53.8
0.125	2.2	1.2	52.6
0.063			
Schale	97.8	52.6	
Summe	185.8	100.0	
Siebverlust			

Prüfung DIN 18 123 - 7

allgemeine Angaben zur Siebanalyse

Datum : 12.04.2011
 Person : Marz
 Trockenmasse [g] : 185.8
 Größtkorn [mm] :
 Kornform :

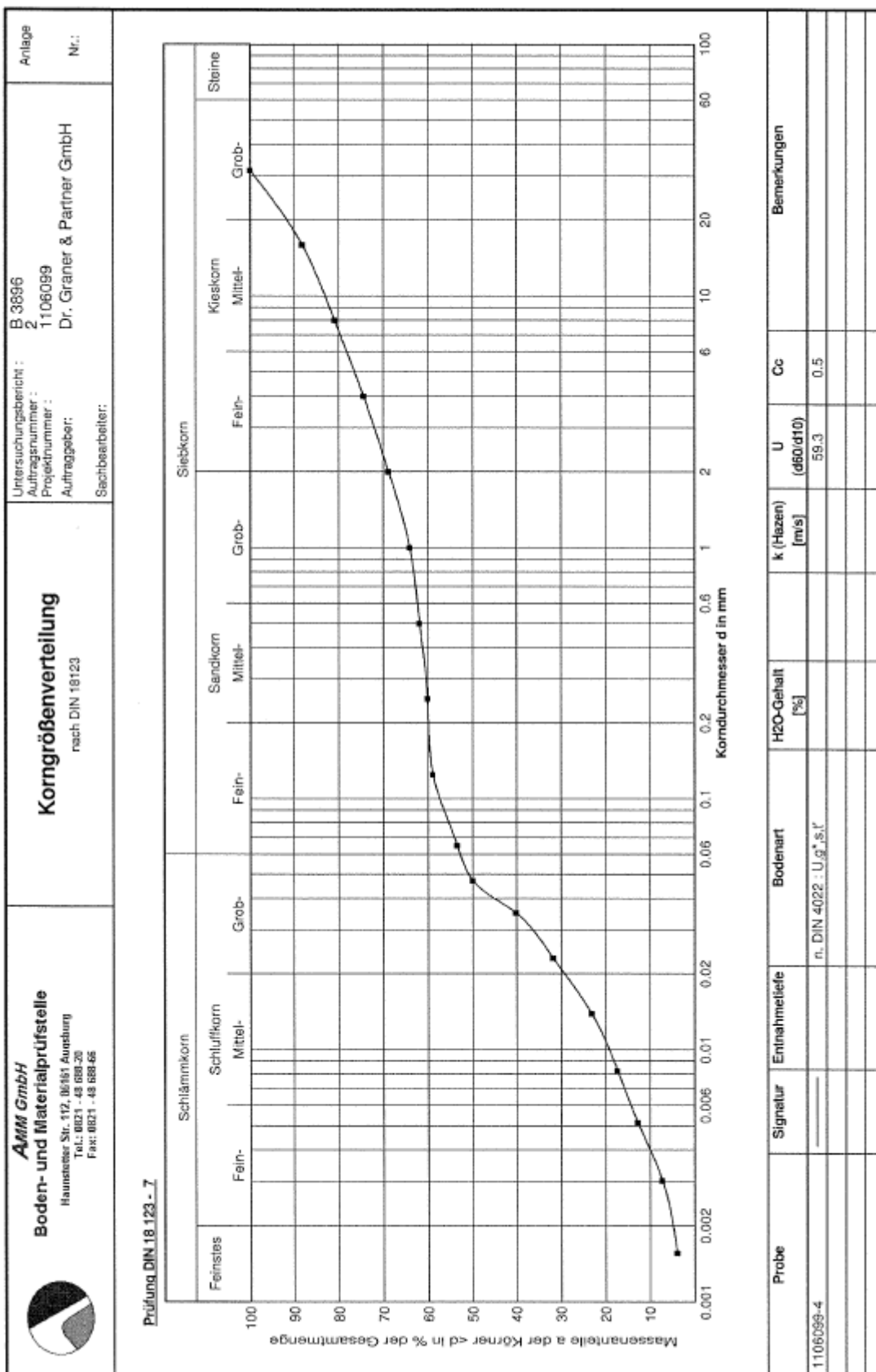
allgemeine Angaben zur Sedimentation

Datum : 18.05.2011
 Person : Schuster
 Trockenmasse [g] : 33.1
 Korndichte [g/cm³] : 2.680
 Ärometer : 8873
 Dispergierungsmittel : Natriumpyrophosphat
 Meniskuskorrektur : 1.10
 100% Lesung : 20.7
 Hilfswert : 4.82

Sedimentation

Zeit- spanne	Ärometer Ablesung R' [g]	Temperatur T [°C]	Korndurch- messer d [mm]	R = R' + Cm		Schlamm- probe a [%]	Gesamt- probe a tot [%]
				R	R + CT		
30'	17.1	22.8	0.0673	18.2	18.8	90.8	47.8
1'	15.1	22.8	0.0489	16.2	16.8	81.1	42.7
2'	12.6	22.8	0.0358	13.7	14.3	69.1	36.4
5'	9.0	22.8	0.0237	10.1	10.7	51.7	27.2
15'	6.0	22.8	0.0141	7.1	7.7	37.3	19.6
45'	3.6	22.8	0.0084	4.7	5.3	25.7	13.5
2h	2.1	22.8	0.0052	3.2	3.8	18.5	9.7
6h	0.5	23.2	0.0030	1.6	2.3	11.2	5.9
24h	0.1	21.4	0.0016	1.2	1.5	7.3	3.9

Bemerkungen :



 AMM GmbH Boden- und Materialprüfstelle Haassteiner Str. 112, 86161 Augsburg Tel.: 0821 - 48 688 20 Fax: 0821 - 48 688 66	Korngrößenverteilung nach DIN 18123	Anlage Nr.:																																																																																																																								
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2 Appendix: Additional data on species and effects for control and treatments

2.1 Abundances of soil organisms

Table Appendix 1: Counts and Abundances of Collembolans in the whole study [1] and for the different treatments of study [1]

species	Σ counts	control	Imidacloprid		Lindane		Abundance [%]
			low	high	low	high	
Parisotoma notabilis	450	419	16	1	7	7	12.4
Isotoma anglicana	419	406	5	2	5	1	11.5
Brachystomella parvula	386	177	4	2	194	9	10.6
Entomobrya lanuginosa	378	159	98	48	49	24	10.4
Lepidocyrtus cyaneus	350	245	59	39	3	4	9.6
Lepidocyrtus lanuginosus	311	187	61	40	16	7	8.5
Sminthurinus aureus	311	255	20	8	26	2	8.5
Bourletiella hortensis	181	47	25	35	42	32	5.0
Sphaeridia pumilis	167	94	21	42	10	.	4.6
Entomobrya multifasciata	124	52	37	25	7	3	3.4
Protaphorura spec.	84	22	27	34	.	1	2.3
Deuterosminthurus pallipes	78	19	15	10	20	14	2.1
Folsomia quadrioculata	75	72	.	1	1	1	2.1
Isotomidae spec.	48	43	1	1	3	.	1.3
Entomobryidae spec.	40	29	4	7	.	.	1.1
Symphyleona spec.	38	21	3	4	8	2	1.0
Mesaphorura spec.	35	28	3	2	1	1	1.0
Collembola indet.	24	12	2	.	9	1	0.7
Friesea truncata	18	16	1	.	1	.	0.5
Isotomurus fucicola/graminis	13	11	1	.	1	.	0.4
Entomobrya spec.	12	7	3	.	1	1	0.3
Mesaphorura krausbaueri group	11	10	.	.	1	.	0.3
Mesaphorura macrochaeta	9	8	1	.	.	.	0.2
Poduromorpha spec.	9	4	2	.	3	.	0.2
Deuterosminthurus spec.	7	2	1	1	2	1	0.2
Folsomides parvulus	7	7	.	.	.	.	0.2
Isotoma viridis	7	4	3	.	.	.	0.2
Onychiuridae spec.	6	2	2	1	.	1	0.2
Sminthurus viridis	6	2	2	.	1	1	0.2
Stenaphorura quadrispina	6	3	.	.	2	1	0.2
Lepidocyrtus spec.	4	1	.	3	.	.	0.1
Folsomia spec.	3	3	.	.	.	.	0.1
Onychiurinae spec.	3	2	.	1	.	.	0.1
Desoria spec.	2	.	.	.	2	.	0.1
Folsomia fimetaria	2	1	1	.	.	.	0.1
Folsomia spec.	2	2	.	.	.	.	0.1
Friesea spec.	2	1	1	.	.	.	0.1
Isotomurus graminis	2	1	.	1	.	.	0.1
Lepidocyrtus lignorum	2	1	1	.	.	.	0.1
Bourletiellidae spec.	1	.	1	.	.	.	0.03
Entomobryinae spec.	1	.	.	1	.	.	0.03
Friesea truncata/mirabilis	1	1	.	.	.	.	0.03
Heterosminthurus bilineatus	1	1	.	.	.	.	0.03
Isotoma spec.	1	1	.	.	.	.	0.03
Pseudosinella alba	1	1	.	.	.	.	0.03
Pseudosinella spec.	1	1	.	.	.	.	0.03
Stenaphorura denisi	1	1	.	.	.	.	0.03
Tomocerus vulgaris	1	.	1	.	.	.	0.03
Tullbergiinae spec.	1	.	.	.	1	.	0.03
total sum	3642	2381	422	309	416	114	

Table Appendix 2: Counts and Abundances of Oribatid mites in the whole study [1] and for the different treatments of study [1]

species	Σ counts	control	Imidacloprid		Lindane		Abundance
			low	high	low	high	[%]
Liebstadia similis	1219	494	313	370	27	15	73.6
juvenile	263	125	54	70	11	3	15.9
Scheloribates laevigatus	48	7	13	8	15	5	2.9
Eupelops occultus	38	27	5	6	.	.	2.3
Banksinoma lanceolata	18	7	6	5	.	.	1.1
Ramusella clavipectinata	16	5	1	2	5	3	1.0
Galumna obvia	15	5	3	7	.	.	0.9
Minunthozetes semirufus	13	5	4	3	1	.	0.8
Punctoribates punctum	8	1	2	4	.	1	0.5
Pantelozetes paolii	3	2	1	.	.	.	0.2
Achipteria coleoprata	2	1	.	1	.	.	0.1
Galumna alata	2	.	2	.	.	.	0.1
Oppiella (Oppiella) nova	2	1	1	.	.	.	0.1
Scutovertex minutus	2	.	1	.	.	1	0.1
Tectocephus velatus	2	1	.	.	.	1	0.1
Ctenobelba pectinigera	1	.	1	.	.	.	0.1
Gustavia microcephala	1	1	.	.	.	.	0.1
Oppiella (Oppiella) falcata	1	.	.	.	1	.	0.1
Scheloribates latipes	1	1	.	.	.	.	0.1
Suctobelba ssp.	1	1	.	.	.	.	0.1
total sum	1656	684	407	476	60	29	

Table Appendix 3: Counts and Abundances of Enchytraeids in the whole study [1] and for the different treatments of study [1]

species	Σ counts	control	Imidacloprid		Lindane		Abundance
			low	high	low	high	[%]
Achaeta "dzwiloi"	1580	262	132	176	441	569	34.9
Buchholzia appendiculata	113	35	12	8	20	38	2.5
Cognettia glandulosa	5		3		1	1	0.1
Enchytraeus norvegicus	13	1	2	1	3	6	0.3
Enchytraeus sp. GRAN	229	41	38	62	42	46	5.1
Enchytraeus sp. PALE	312	77	69	45	40	81	6.9
Enchytronia parva s.l.	372	84	46	32	92	118	8.2
Fridericia sp.	170	58	18	16	40	38	3.8
Fridericia benti	29	15	4	3	3	4	0.6
Fridericia bisetosa	129	43	20	13	30	23	2.9
Fridericia bulboides	160	58	20	22	27	33	3.5
Fridericia connata	630	227	126	56	127	94	13.9
Fridericia dura c.f.	39	9	1	9	12	8	0.9
Fridericia galba	228	75	31	35	41	46	5.0
Fridericia paroniana	94	48	6	8	9	23	2.1
Fridericia sylvatica	59	25	11	8	7	8	1.3
Fridericia ulrikae	246	85	56	23	43	39	5.4
Henlea perpusilla	65	20	4	7	18	16	1.4
Marionina communis	51	17	9	9	9	7	1.1
Gesamtsumme	4524	1180	608	533	1005	1198	100.0

Table Appendix 4: Counts and Abundances of Lumbricids in the whole study [1] and for the different treatments of study [1]

species	Σ counts	control	Imidacloprid		Lindane		Abundance [%]
			low	high	low	high	
Aporrectodea / Allolobophora spec.	1073	205	445	310	84	29	42.1
Aporrectodea caliginosa	543	114	179	181	52	17	21.3
Aporrectodea rosea	73	21	23	22	3	4	2.9
Lumbricus castaneus	32	6	12	12	2		1.3
Lumbricus rubellus	55	22	16	14	1	2	2.2
Lumbricus sp.	441	110	153	124	31	23	17.3
Lumbricus terrestris	124	35	40	22	10	17	4.9
Octolasion sp.	135	21	56	39	11	8	5.3
Octolasion cyaneum	70	14	34	13	6	3	2.7
Octolasion juvenile	1			1			0.0
total sum	2547	548	958	738	200	103	100.0

Table Appendix 5: Counts and Abundances of Lumbricids in the whole study [3] and for the different treatments of study [3]

species	Σ counts	Control	Carbendazim		Abundance [%]
			low	high	
Aporrectodea / Allolobophora spec.	861	534	237	90	50.6
Aporrectodea caliginosa	255	180	55	20	15.0
nicht bestimmbar	230	137	68	25	13.5
Lumbricus sp.	152	135	15	2	8.9
Octolasion sp.	56	31	15	10	3.3
Aporrectodea rosea	49	39	8	2	2.9
Octolasion cyaneum	41	26	9	6	2.4
Lumbricus castaneus	22	21	1		1.3
Lumbricus terrestris	15	13	1	1	0.9
Lumbricus rubellus	10	10			0.6
Aporrectodea limicola	6	4		2	0.4
Octolasion lacteum	3	3			0.2
Allolobophora chlorotica	1	1			0.1
total sum	1701	1134	409	158	100.0

2.2 Further results of statistical analyses

Table Appendix 6: Table of statistical analysis (Williams t-test) of the effects of Lindane in study [1]. Endpoint is the sum of collembolans for different soil layers (0-C) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, grey: no sampling,

Sampling date	Layer	O Surface			A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			all (without surface)		
		Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD
day 14	Conc.	*	*	51	*	*	59	*	*	64	-	-	81	*	*	58
day 42		*	*	56	*	*	46	*	*	63	*	*	60	*	*	52
day 140		-	*	62	-	*	64	*	*	59	*	*	74	-	*	57
day 189					*	*	58	*	*	56				*	*	55
day 364		*	*	46	-	*	54	*	*	62	*	*	63	*	*	49

Table Appendix 7: Table of statistical analysis (Williams t-test) of the effects of Imidacloprid in study [1]. Endpoint is the sum of collembolans for different soil layers (0-C) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, grey: no sampling,

Sampling date	Layer	Q Surface			A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			all (without surface)		
	Conc.	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD
day 14		-	*	57	*	*	58	*	*	67	-	-	88	*	*	55
day 42		*	*	35	*	*	49	*	*	50	*	*	58	*	*	44
day 140		-	*	75	-	-	63	-	-	79	-	-	84	-	-	55
day 189					-	-	68	*	*	59				*	*	63
day 364		*	*	53	-	*	66	-	-	76	*	*	66	*	*	57

Table Appendix 8: Table of statistical analysis (Williams t-test) of the effects of Lindane in study [1]. Endpoint is the sum of oribatid mites for different soil layers (A-C) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, grey: no sampling,

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			all		
	Conc.	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD
day 14		*	*	65	-	-	111	-	-	88	*	*	60
day 42		*	*	52	-	*	72	-	-	n.c.	*	*	43
day 140		*	*	42	-	-	146	-	-	-	*	*	43
day 189		*	*	64	*	*	84			-	*	*	64
day 364		*	*	57	-	-	141	*	*	91	*	*	58

Table Appendix 9: Table of statistical analysis (Williams t-test) of the effects of Imidacloprid in study [1]. Endpoint is the sum of oribatid mites for different soil layers (A-C) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, grey: no sampling,

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			all		
	Conc.	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD
day 14		-	-	67	-	-	102	-	-	105	-	-	54
day 42		-	-	49	-	-	73	-	-	n.c.	-	-	48
day 140		*↑	*↑	44	-	-	183	-	-	n.c.	*↑	*↑	45
day 189		-	-	66	-	-	102			-	-	-	66
day 364		-	-	45	-	-	139	-	-	127	-	-	43

Table Appendix 10: Table of statistical analysis (Williams t-test) of the effects of Lindane in study [1]. Endpoint is the sum of enchytraeids for different soil layers (A-C) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum; grey: no sampling, arrow: increase in abundance

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			all		
	Conc.	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD
day 14		*↑	*↑	65	-	-	51	-	-	79	-	*↑	47
day 42		*↑	*↑	62	*↑	*↑	73	-	*↑	85	*↑	*↑	54
day 140		-	-	84	-	-	97	-	-	87	-	-	77
day 189		-	-	89	-	-	79			-	-	-	80
day 364		-	-	82	-	-	89	-	-	107	-	-	77

Table Appendix 11: Table of statistical analysis (Williams t-test) of the effects of Imidacloprid in study [1]. Endpoint is the sum of enchytraeids for different soil layers (A-C) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, grey: no sampling, arrow: increase in abundance

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			all		
	Conc.	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD
day 14		-	-	60	-	-	36	-	-	73	-	-	34
day 42		-	-	65	* ↑	* ↑	70	-	-	78	-	-	57
day 140		-	-	76	-	-	87	-	-	80	-	-	69
day 189		-	-	90	-	-	77				-	-	79
day 364		-	-	66	-	-	91	-	-	96	-	-	63

Table Appendix 12: Table of statistical analysis (Williams t-test) of the effects of Lindane in study [1]. Endpoint is the sum of lumbricids for different soil layers (A-E) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum; arrow: increase in abundance

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			D: 10-20 cm			E: 20-40 cm			all		
	Conc.	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD	Lindane low	Lindane high	MDD
day 14		-		52	-		48	-		38	-		34	-		44	-		18
day 140		-		85	-		69	-		30	-		37	-		54	-		39
day 364		-	-	63	-	-	61	-	-	52	-	-	68	-	* ↑	42	-	-	44

Table Appendix 13: Table of statistical analysis (Williams t-test) of the effects of Imidacloprid in study [1]. Endpoint is the sum of lumbricids for different soil layers (A-E) and at different sampling dates (day 14-364). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, arrow: increase in abundance

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			D: 10-20 cm			E: 20-40 cm			all		
	Conc.	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD	Imida low	Imida high	MDD
day 14		-		53	-		62	-		32	-		45	-		47	-		16
day 140		-		87	-		59	-		39	* ↑		35	-		45	-		31
day 364		*	*	52	-	*	51	-	-	53	-	-	69	-	-	46	*	*	35

Table Appendix 14: Table of statistical analysis (Williams t-test) of the effects of Carbendazim in study [3]. Endpoint is the sum of lumbricids for different soil layers (A-E) and at different sampling dates (day 16-148). *: significant difference (p-value < 0.05); MDD: Minimum Detectable Minimum, arrow: increase in abundance

Sampling date	Layer	A: 0-2.5 cm			B: 2.5-5 cm			C: 5-10 cm			D: 10-20 cm			E: 20-40 cm			all		
	Conc.	Carb low	Carb high	MDD	Carb low	Carb high	MDD	Carb low	Carb high	MDD	Carb low	Carb high	MDD	Carb low	Carb high	MDD	Carb low	Carb high	MDD
day 16		*	*	57	-	-	66	-	*	34	-	*	61	-	-	159	*	*	30
day 114		*	*	69	-	*	76	-	*	69	*	*	61	*	*	64	*	*	57
day 148		*	*	68	*	*	66	*	*	57	-	-	86	*	*	65	*	*	63

Table Appendix 15: Effects of Lindane on the species and species groups of collembolans for different soil layers sampling dates. – means the database is not sufficient for calculation; 20000 and 20000+: no effect could be detected; 7500: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer	all					O				A					B					C			
days after application	14	42	140	189	364	14	42	140	364	14	42	140	189	364	14	42	140	189	364	14	42	140	364
Entomobryomorpha	0	20000 +	0	0	0	-	-	-	-	0	0	0	0	0	-	-	-	-	-	-	-	-	-
Oxychiridae	20000	20000 +	7500	0	0	-	-	-	-	20000	20000 +	20000	20000	0	-	-	-	-	-	-	-	-	-
Poduromorpha	20000	0	20000	7500	20000	-	-	-	-	20000	0	20000	20000	20000	-	-	-	-	-	-	-	-	-
Symphyleona	0	0	20000	0	7500	-	-	-	-	0	0	20000	0	7500	-	-	-	-	-	-	-	-	-
Bourletiella hortensis	-	-	-	-	-	-	20000	-	20000 +	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Bourletiellidae spec.	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Brachystomella parvula	20000	20000	20000	20000	20000	0	0	20000	20000	20000	20000	20000	20000	20000	-	20000	-	20000	-	-	-	-	-
Collembola indet.	20000	20000	-	-	20000	-	20000	-	-	20000	-	-	-	20000	-	-	-	-	20000	20000 +	20000	-	-
Desoria spec. 1	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Deuterosminthurus pallipes	-	-	-	-	-	20000	20000 +	20000	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Deuterosminthurus spec.	-	-	-	-	-	-	20000	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Entomobrya lanuginosa	0	20000	20000	20000	20000	20000	0	20000	20000 +	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000	20000
Entomobryinae spec.	-	-	-	-	-	-	20000 +	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Entomobrya spec.	-	20000	20000	-	-	-	-	-	-	-	20000	20000	-	-	-	-	-	-	-	-	-	-	-
Entomobrya multifasciata	20000	0	20000	-	20000	0	0	20000	20000	20000	0	20000	-	20000	-	20000	20000	-	-	-	20000	-	20000
Entomobryidae spec.	-	-	0	20000	-	-	0	20000	-	-	-	0	20000	-	-	-	-	-	-	-	-	-	-
Folsomia fimetaria	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-
Folsomides parvulus	-	-	-	-	0	-	-	-	-	-	-	-	-	20000	-	-	-	-	20000	-	-	-	-
Folsomia quadriculata	0	0	0	0	0	-	-	-	-	20000 +	0	20000	20000	20000	0	-	20000	0	0	20000	-	-	-
Folsomia spec. 1	20000	-	-	20000	-	-	-	-	-	-	-	-	20000	-	20000	-	-	-	-	-	-	-	-
Folsomia spec.	20000	-	-	-	20000	-	-	-	-	-	-	-	-	-	20000	-	-	-	20000	-	-	-	-
Friesea spec.	-	20000	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-
Friesea truncata	20000	20000	20000	20000	-	-	20000	20000	-	20000	20000	20000	-	-	-	20000	20000	20000	20000	-	20000	-	20000
Friesea truncata/ mirabilis	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	20000	-	-	-	-
Heterosminthurus bilineatus	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Isotoma anglicana	-	0	20000	20000	7500	0	20000 +	0	0	-	0	20000	-	7500	-	20000	20000	20000	-	-	20000	20000	20000
Isotomurus fucicola/ graninis	-	-	-	-	20000	-	-	-	20000	20000	-	-	-	20000	-	-	-	-	-	-	-	-	-
Isotomurus graninis	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Isotoma spec.	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Isotomidae spec.	20000	-	-	-	20000	20000	0	20000	20000	-	-	-	-	20000	-	-	-	-	-	-	-	-	20000
Isotoma viridis	-	-	-	-	-	20000	20000	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-
Lepidocyrtus cyaneus	0	0	0	20000 +	20000	-	0	20000 +	20000 +	20000	0	0	0	20000	-	-	20000	20000 +	20000	20000	20000	-	20000
Lepidocyrtus lanuginosus	20000	0	0	0	20000	-	20000 +	0	0	-	20000	0	0	20000	20000	20000	20000	20000 +	-	-	20000	20000	20000
Lepidocyrtus lignorum	-	20000	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-
Lepidocyrtus spec.	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Mesaphorura krausbaueri group	-	20000	20000	-	20000	-	-	-	-	-	20000	20000	-	-	-	20000	-	-	-	-	20000	-	20000
Mesaphorura macrochaeta	-	20000	20000	20000	20000	-	-	-	-	-	-	-	-	-	-	20000	20000	20000	-	-	-	-	20000
Mesaphorura spec.	20000	20000	20000	20000	0	-	-	-	-	-	-	20000	20000	-	20000	-	20000	20000	-	20000	20000	20000 +	0
Oxychiridae spec.	20000 +	20000	-	-	-	-	-	-	-	20000	-	-	-	-	20000	-	-	-	-	-	20000 +	20000	-
Oxychirinae spec.	20000	-	-	-	-	-	-	-	-	0	-	-	-	0	-	-	-	-	-	20000	-	-	-
Parisotoma notabilis	0	20000 +	20000	0	0	20000	-	-	-	20000	0	20000	0	20000	7500	20000 +	20000	20000	20000	20000	20000 +	20000	-
Poduromorpha spec.	20000	-	-	-	20000	-	20000	-	-	-	-	-	-	0	-	-	-	-	-	20000	-	-	-
Protaphorura spec.	20000	20000 +	20000	20000	0	-	-	-	-	20000	20000 +	20000	20000	-	20000	20000	-	20000	20000	-	-	-	20000
Pseudosinella alba	20000	-	-	-	-	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-
Pseudosinella spec.	-	-	20000	-	-	-	-	-	-	20000	-	-	-	-	-	-	20000	-	-	-	-	-	-
Sminthurinus aureus	20000	0	20000	20000	20000	20000 +	0	0	0	20000	20000	20000	20000	-	-	20000	-	-	-	-	-	-	-
Sminthurus viridis	20000	-	-	-	-	-	20000	-	20000	20000	-	-	-	0	-	-	-	-	-	-	-	-	-
Sphaeridia pumilis	20000	0	-	20000	0	20000	0	-	0	-	0	-	20000	-	-	-	-	-	-	-	-	-	-
Stenaphorura quadrispina	20000	20000 +	20000	20000	-	-	-	-	-	20000	-	20000	-	-	-	-	20000	20000	-	-	20000	20000 +	20000
Stenaphorura denisi	20000	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-
Symphyleona spec.	20000	20000	-	-	-	20000	20000	20000 +	20000	20000	20000	-	-	-	20000	-	-	-	-	-	20000	-	-
Tullbergiinae spec.	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table Appendix 16: Effects of Lindane on oribatid mites species for different soil layers sampling dates. – means the database is not sufficient for calculation; 20000 and 20000+: no effect could be detected; 7500: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer day after application	all					A					B					C			
	14	42	140	189	364	14	42	140	189	364	14	42	140	189	364	14	42	140	364
<i>Achipteria coleoptrata</i>	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	20000	-	-	-
<i>Banksinoma lanceolata</i>	-	20000	20000	20000	20000	-	20000	20000	-	20000	-	-	-	20000	-	-	-	-	-
<i>Otenobelba pectinigera</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>Eupelops occultus</i>	-	20000	0	0	0	-	20000	0	0	0	-	-	-	-	-	-	-	-	-
<i>Galuma alata</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>Galuma obvia</i>	-	-	20000	20000	-	-	-	20000	-	-	-	-	-	20000	-	-	-	-	-
<i>Gustavia microcephala</i>	20000	-	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-
<i>Liebstadia similis</i>	20000 +	0	0	0	0	20000 +	0	0	0	0	20000	7500	20000	20000	20000 +	20000 + 20000 +	-	-	0
<i>Minuthozetes seminifus</i>	20000	20000	-	-	-	20000	20000	-	-	-	20000	20000	-	-	-	20000	-	-	-
<i>Oppeia (Oppeia) falcata</i>	20000	-	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-
<i>Oppeia (Oppeia) nova</i>	-	20000	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-
<i>Pantelozetes padii</i>	-	-	-	20000	20000	-	-	-	-	-	-	-	-	20000	20000	-	-	-	-
<i>Punctobates punctum</i>	-	-	-	-	20000 +	-	-	-	-	20000	-	-	-	-	20000 +	-	-	-	-
<i>Ramusella davipectinata</i>	20000	20000	-	-	-	20000	0	-	-	-	20000 +	-	-	-	-	20000	20000	-	-
<i>Scheloribates laevigatus</i>	20000 +	20000	20000 +	20000	20000	-	20000	20000 +	20000	20000	20000 +	-	-	-	20000	-	-	-	-
<i>Scheloribates latipes</i>	20000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	20000	-	-	-
<i>Suctobelba spec.</i>	20000	-	-	-	-	-	-	-	-	-	20000	-	-	-	-	-	-	-	-
<i>Tectocephus velatus</i>	20000	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	-	-	-	-
juvenile	20000	7500	20000	0	0	20000	0	20000	0	0	20000	20000	20000	-	20000 +	-	-	-	-
unknown	20000	20000	-	-	-	20000	20000	-	-	-	-	20000	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table Appendix 17: Effects of Lindane on the enchtraeid species for different soil layers sampling dates. – means the database is not sufficient for calculation; 20000 and 20000+: no effect could be detected; 7500: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test) ; +: increase in abundance

layer days after application	all					A					B					C			
	14	42	140	189	364	14	42	140	189	364	14	42	140	189	364	14	42	140	364
<i>Achaeta "dzwilli"</i>	0+	20000	20000	20000	20000+	20000	20000	20000	20000	20000+	0+	20000	20000+	0	20000+	20000+	7500+	20000	20000
<i>Buchholzia appendiculata</i>	20000+	20000	20000+	20000	20000	20000+	20000	20000+	20000	20000+	20000+	20000	7500+	20000	20000	20000	20000	-	20000
<i>Cognettia glandulosa</i>	20000	-	-	-	-	20000	-	-	-	-	-	-	-	-	-	20000+	-	-	-
<i>Enchytraeus norvegicus</i>	-	-	20000+	20000	20000+	-	-	7500+	-	20000	-	-	-	20000	20000+	-	-	20000	-
<i>Enchytronia parva s.l.</i>	0+	20000+	7500+	20000	20000+	20000	20000+	7500+	20000	20000	0+	20000+	7500+	20000	20000+	20000	20000+	20000	7500+
<i>Enchytraeus sp. GRAN</i>	20000	7500+	7500+	20000	20000	-	7500+	7500+	20000	20000	20000	20000	20000	20000	-	20000	20000	20000	20000
<i>Enchytraeus sp. PALE</i>	20000+	20000+	20000	20000+	20000+	20000+	20000+	20000+	20000+	20000+	20000	20000+	20000	20000+	7500+	20000+	20000+	20000+	20000
<i>Fridericia benti</i>	20000+	20000+	20000	20000	20000	20000+	20000+	20000	-	-	20000+	-	20000	20000	20000	-	-	-	20000
<i>Fridericia bisetosa</i>	20000+	20000	20000	20000	20000	20000+	20000	20000+	20000	20000	20000+	20000	20000	20000	20000	20000+	-	20000	20000
<i>Fridericia bulboides</i>	20000	20000+	20000+	20000	20000	20000	20000+	20000+	20000	20000	20000	20000	20000	-	20000	20000	20000	-	20000
<i>Fridericia connata</i>	20000	7500+	20000	20000	20000	20000	20000+	20000	7500	20000	20000	20000	20000	20000	-	20000	20000	-	-
<i>Fridericia dura c.f.</i>	20000+	20000	7500+	20000	20000	20000+	20000	20000+	-	20000	20000+	20000	-	20000	-	-	-	20000	-
<i>Fridericia galba</i>	20000+	20000	20000+	20000+	20000	20000+	20000	20000+	20000	20000+	20000+	20000+	20000	20000+	20000	20000	20000	7500+	20000
<i>Fridericia paroniana</i>	20000+	20000+	7500	20000	20000	20000	20000+	20000	20000	20000	20000	20000+	20000	20000	-	20000+	-	-	-
<i>Fridericia sp.</i>	20000	0+	20000+	-	20000	20000	20000	20000+	-	20000	20000	20000	20000	-	20000	20000+	20000+	-	20000
<i>Fridericia sylvatica</i>	20000+	20000+	20000	20000	20000+	20000+	20000+	20000	20000	20000+	20000+	-	20000	20000	-	20000	20000+	-	-
<i>Fridericia ulrikae</i>	20000	7500+	20000+	20000+	20000	20000	7500+	20000+	20000+	20000	20000+	20000+	20000	20000	20000	20000	20000+	20000	20000
<i>Henlea perpusilla</i>	20000	20000	7500+	20000	-	20000+	20000	20000+	20000	-	20000+	20000+	7500+	20000	-	20000	20000	-	-
<i>Marionina communis</i>	20000	20000	20000	20000+	-	20000+	20000	20000	20000	-	20000	-	20000	20000+	-	0	-	-	-

Table Appendix 18: Effects of Lindane on the lumbricid species for different soil layers sampling dates. – means the database is not sufficient for calculation; 20000 and 20000+: no effect could be detected; 7500: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer	all	A	B	C	D	E
days after application	364	364	364	364	364	364
<i>Aporrectodea</i> / <i>Allolobophora</i> spec.	20000	20000	20000	20000	20000+	7500+
<i>Aporrectodea caliginosa</i>	20000	20000	20000+	20000+	20000+	20000+
<i>Aporrectodea rosea</i>	20000+	20000+	20000+	20000	20000+	-
<i>Lumbricus castaneus</i>	20000	20000	-	-	-	20000+
<i>Lumbricus rubellus</i>	20000	20000+	20000	-	-	-
<i>Lumbricus</i> sp.	20000+	20000	20000+	20000+	20000+	20000+
<i>Lumbricus terrestris</i>	20000	20000	-	-	20000+	20000
<i>Octolasion cyaneum</i>	20000+	20000	20000	20000	20000+	20000+
<i>Octolasion</i> sp.	20000	20000	20000	20000	20000+	20000

Table Appendix 19: Effects of Imidacloprid on the species and species groups of collembolans for different soil layers sampling dates. – means the database is not sufficient for calculation; 2000 and 2000+: no effect could be detected; 750: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer days after application	all					O					A					B					C				
	14	42	140	189	364	14	42	140	364		14	42	140	189	364	14	42	140	189	364	14	42	140	189	364
Entomobryomorpha	750	0	2000	2000+	0	-	-	-	-		750	0	2000	2000+	0	-	-	-	-	-	-	-	-	-	-
Oxyduriidae	2000	2000+	2000+	2000+	2000	-	-	-	-		2000+	2000	2000+	2000+	2000	-	-	-	-	-	-	-	-	-	-
Poduromorpha	2000	750	2000	750	2000	-	-	-	-		2000	2000	2000	2000	2000	-	-	-	-	-	-	-	-	-	-
Symphyleona	2000+	0	2000	2000	2000+	-	-	-	-		2000+	0	2000	2000	2000+	-	-	-	-	-	-	-	-	-	-
Bourlettiella hortensis	-	-	-	-	-	-	2000	-	2000+		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Bourlettiellidae spec.	-	-	-	-	-	2000	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Brachystomella parvula	2000	2000	2000	2000	2000	0	0	750	2000+		2000	2000	2000	2000	2000	-	2000	-	2000	-	-	-	-	-	-
Collembola indet.	2000	2000	-	-	2000	-	2000	-	-		2000	-	-	-	2000	2000	-	-	2000	-	-	2000	-	-	-
Desoria spec.	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Deuterosminthurus pallipes	-	-	-	-	-	-	2000+	2000	2000		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Deuterosminthurus spec.	-	-	-	-	-	2000+	2000	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Entomobrya lanuginosa	2000	2000	2000	2000+	2000	2000	2000	2000	2000+		2000	2000	2000	2000+	2000	2000	2000	2000	2000+	-	2000+	-	2000	-	2000
Entomobryinae spec.	-	-	-	-	-	-	-	-	2000+		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Entomobrya spec.	2000	2000	2000	-	-	-	2000	2000	-		2000	2000	2000	-	-	-	-	-	-	-	-	-	-	-	-
Entomobrya multifasciata	2000	750	2000+	-	2000	2000	2000	2000+	2000+		2000	750	2000+	-	2000+	-	2000	2000	-	-	2000	2000	-	-	2000
Entomobryidae spec.	-	-	2000+	2000+	-	-	2000+	2000+	-		-	0	2000+	-	-	-	-	-	-	-	-	-	2000+	-	-
Folsomia fimetaria	-	2000	2000	-	-	-	-	-	-		-	2000	-	-	-	-	-	2000	-	-	-	-	-	-	-
Folsomides parvulus	-	-	-	-	0	-	-	-	-		-	-	-	-	2000	-	-	-	-	2000	-	-	-	-	-
Folsomia quadrioculata	2000+	0	0	0	0	-	-	-	-		2000	0	2000	2000	2000	2000+	-	2000	0	0	2000	-	-	-	-
Folsomia spec. 1	2000	-	-	2000	-	-	-	-	-		-	-	-	2000	-	2000	-	-	-	-	-	-	-	-	-
Folsomia spec.	2000	-	-	-	2000	-	-	-	-		-	-	-	-	-	2000	-	-	-	2000	-	-	-	-	-
Friesia spec.	-	2000	-	2000	-	-	-	-	-		-	2000	-	-	-	-	-	-	2000	-	-	-	-	-	-
Friesia truncata	2000	2000	2000	2000	-	-	2000	2000	-		-	2000	2000	-	-	-	2000	2000	2000	-	2000	-	2000	-	-
Friesia truncata/ mirabilis	-	-	-	-	2000	-	-	-	-		-	-	-	-	-	-	-	-	-	2000	-	-	-	-	-
Heterosminthurus bilineatus	-	-	-	-	-	-	-	2000	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Isotoma anglicana	-	0	2000	2000	750	0	0	0	0		-	0	2000	-	750	-	2000	2000	2000	-	-	2000	2000	-	-
Isotomurus fucicola/ graminis	-	-	-	-	2000	-	-	-	2000		-	-	-	-	2000	-	-	-	-	-	-	-	-	-	-
Isotomurus graminis	-	-	-	-	-	2000	-	2000+	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Isotoma spec.	-	-	-	-	-	-	2000	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Isotomidae spec.	2000	-	-	-	2000	2000	2000+	2000	2000		2000	-	-	-	2000	-	-	-	-	-	-	-	-	-	2000
Isotoma viridis	-	-	-	-	2000	2000	2000	-	-		-	-	-	-	2000	-	-	-	-	-	-	-	-	-	-
Lepidocyrtus cyaneus	750	750	2000+	2000	2000	-	0	2000	2000+		2000	750	2000+	2000	2000	-	-	2000+	0	2000	2000	2000	2000	-	2000
Lepidocyrtus lanuginosus	2000	2000+	2000	2000+	2000+	-	2000	2000	0		2000	2000+	2000	2000+	2000+	2000	2000	2000	2000+	-	-	2000	2000	-	2000
Lepidocyrtus lignorum	2000	2000	-	-	-	-	-	-	-		-	2000	2000	-	-	-	-	-	-	-	-	-	-	-	-
Lepidocyrtus spec.	2000+	-	-	-	-	-	2000	2000+	-		2000+	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Mesaphorura krausbaueri group	-	2000	2000	-	2000	-	-	-	-		-	2000	2000	-	-	-	2000	-	-	-	-	2000	-	-	2000
Mesaphorura macrochaeta	-	2000	2000	2000	2000	-	-	-	-		-	-	-	-	-	-	2000	2000	2000	-	-	-	-	-	2000
Mesaphorura spec.	2000	2000+	2000	2000	0	-	-	-	-		-	-	2000	2000	-	2000	-	2000	2000	-	2000	2000+	2000	-	0
Oxyduriidae spec.	2000	2000+	2000	-	-	-	-	-	-		-	-	2000	-	-	2000	-	-	-	-	-	2000+	-	-	-
Oxyduriinae spec.	2000+	-	-	-	-	-	-	-	-		2000+	-	-	-	-	-	-	-	-	-	-	2000	-	-	-
Parisotoma notabilis	0	0	2000	0	0	2000	-	-	-		0	0	2000	0	0	750	2000	2000	2000	2000	2000	2000	-	-	2000
Poduromorpha spec.	2000	-	-	-	2000	-	2000	-	2000		2000	-	-	-	2000	-	-	-	-	2000	-	-	-	-	-
Protaphorura spec.	2000	2000	750 +	750 +	2000	-	-	-	-		-	-	2000+	750 +	2000	2000	2000	750 +	750 +	2000+	-	-	-	-	2000
Pseudosinella alba	2000	-	-	-	-	-	-	-	-		2000	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Pseudosinella spec.	-	-	2000	-	-	-	-	-	-		-	-	-	-	-	-	-	2000	-	-	-	-	-	-	-
Sminthurus aureus	2000+	2000	2000	2000	2000+	750	0	0	0		2000+	2000	2000	2000	2000+	-	2000	-	-	-	-	-	-	-	-
Sminthurus viridis	2000	-	-	-	-	-	2000	2000	2000		2000	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sphaeridia pumilis	2000	0	2000	2000	2000+	2000	0	-	2000		2000	0	2000	2000	2000+	-	-	-	-	-	-	-	-	-	-
Stereophorura quadrispina	2000	-	2000	2000	-	-	-	-	-		-	-	-	-	-	-	-	2000	2000	-	2000	-	-	-	-
Stereophorura densi	2000	-	-	-	-	-	-	-	-		2000	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Symphyleona spec.	2000	2000	-	-	-	2000	2000+	2000	2000		2000	2000	-	-	-	2000	-	-	-	-	-	2000	-	-	-
Tullbergiinae spec.	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Tomocerius vulgaris	-	-	-	-	-	2000	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table Appendix 20: Effects of Imidacloprid on oribatid mites species for different soil layers sampling dates. – means the database is not sufficient for calculation; 2000 and 2000+: no effect could be detected; 750: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer day after application	all					A					B					C			
	14	42	140	189	364	14	42	140	189	364	14	42	140	189	364	14	42	140	364
<i>Achipteria coleoptrata</i>	2000+	-	-	-	-	2000+	-	-	-	-	-	-	-	-	-	2000	-	-	-
<i>Banksinoma lanceolata</i>	-	2000	2000+	2000	2000+	-	2000	2000+	-	2000+	-	-	-	2000	-	-	-	2000+	-
<i>Otenobelba pectinifera</i>	2000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2000	-	-	-
<i>Eupelops occultus</i>	-	2000	2000	2000	2000	-	2000	2000	2000	2000	-	-	-	-	-	-	-	-	-
<i>Galumna alata</i>	2000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2000	-	-	-
<i>Galumna obvia</i>	2000+	2000+	2000	2000+	2000	-	-	2000	2000+	2000+	2000+	2000+	-	2000	2000	-	-	-	-
<i>Gustavia microcephala</i>	2000	-	-	-	-	-	-	-	-	-	2000	-	-	-	-	-	-	-	-
<i>Liebstadia similis</i>	2000	2000+	0 +	2000+	2000+	2000	2000+	0 +	2000+	2000+	2000	2000	2000+	2000+	2000+	2000	-	2000	2000
<i>Minuthozetes seminifus</i>	2000+	2000	2000	-	-	750+	2000	2000	-	-	2000	2000	-	-	-	2000	-	2000	-
<i>Oppeia (Oppeia) falcata</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>Oppeia (Oppeia) nova</i>	-	2000	-	-	-	-	2000	-	-	-	-	-	-	-	-	-	-	-	-
<i>Pantelozetes padii</i>	-	2000	-	2000	2000	-	-	-	-	-	-	2000	-	2000	2000	-	-	-	-
<i>Pantelozetes punctum</i>	2000	2000+	2000+	2000+	2000	2000	2000+	2000+	2000+	2000	-	-	-	-	-	-	-	-	-
<i>Ramusella clavipunctata</i>	2000	2000	-	-	2000+	-	0	-	-	-	2000	2000+	-	-	-	2000	-	-	2000+
<i>Scheloniobates laevigatus</i>	2000	2000	0+	2000+	2000+	2000	2000	2000	2000+	2000+	2000	-	-	2000+	2000	2000	-	2000+	2000
<i>Scheloniobates latipes</i>	2000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2000	-	-	-
<i>Suctobelba</i>	2000	-	-	-	-	-	-	-	-	-	2000	-	-	-	-	-	-	-	-
<i>Tectocephus velatus</i>	2000	-	-	-	-	2000	-	-	-	-	-	-	-	-	-	-	-	-	-
juveniles	2000+	2000+	2000+	2000	2000+	2000+	2000+	2000+	2000	2000+	2000	2000	2000	-	2000+	2000+	-	2000+	2000
unknown	2000	2000	-	-	-	2000	2000	-	-	-	-	2000	-	-	-	-	-	-	-

Table Appendix 21: Effects of Imidacloprid on the enchtraeid species for different soil layers sampling dates. – means the database is not sufficient for calculation; 2000 and 2000+: no effect could be detected; 750: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer day after application	all					A					B					C			
	14	42	140	189	364	14	42	140	189	364	14	42	140	189	364	14	42	140	364
<i>Achaeta "dovillioi"</i>	2000+	2000+	2000	2000+	2000+	2000+	2000+	2000+	2000	2000+	2000	0+	2000	2000+	2000+	2000	750+	2000	2000+
<i>Buchholzia appendiculata</i>	2000+	2000	2000	2000+	2000+	2000	2000	2000	2000	2000+	2000	2000+	2000	2000+	2000	2000+	2000	-	-
<i>Cognettia glandulosa</i>	2000	2000	-	-	-	2000	2000	-	-	-	2000	-	-	-	-	-	-	-	-
<i>Enchytraeus norvegicus</i>	-	-	2000	-	-	-	-	2000	-	-	-	-	-	-	-	-	-	2000	-
<i>Enchytraeus parva s.l.</i>	2000+	2000	2000	2000+	2000	2000+	2000	2000	2000	2000	2000+	2000	2000	2000+	2000	2000	2000	2000	2000
<i>Enchytraeus sp. GRAN</i>	2000+	2000	750+	2000+	750+	2000+	2000	750+	750+	750+	2000	2000+	2000	2000+	2000	2000	2000	2000	750+
<i>Enchytraeus sp. PALE</i>	2000	2000	2000	750+	2000+	2000+	2000	2000+	2000	2000+	2000	2000+	2000	2000+	2000	2000	2000	2000	2000
<i>Fridericia benti</i>	2000	-	2000+	2000	2000	2000	-	2000	-	2000	2000	-	2000	2000	-	2000+	-	2000+	2000
<i>Fridericia bisetosa</i>	2000	2000	2000+	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	-	2000+	-	2000+	2000
<i>Fridericia bulboides</i>	2000	2000	2000+	2000	2000+	2000+	2000	2000+	2000	2000+	2000	2000	2000	2000	2000+	2000	2000	-	2000+
<i>Fridericia connata</i>	2000	2000	750	2000+	2000	2000	2000	750	0	2000	2000	2000	2000	2000+	-	2000+	2000	2000	2000+
<i>Fridericia dura c.f.</i>	2000+	2000+	2000+	2000+	2000+	-	2000	2000+	750+	2000+	0	2000	2000	2000	-	750+	2000+	-	-
<i>Fridericia galba</i>	2000+	2000	2000+	2000+	2000+	2000+	2000	2000+	2000+	2000+	2000	2000	2000	2000+	2000	2000	2000	2000	2000
<i>Fridericia paroniana</i>	2000+	2000+	2000	2000	2000	2000	2000	2000	2000	2000	2000+	-	2000	2000	-	2000+	2000+	-	-
<i>Fridericia sp.</i>	2000	2000+	2000	-	2000+	2000	2000+	2000	-	2000+	2000	2000+	2000	-	2000	2000	2000+	-	2000
<i>Fridericia sylvatica</i>	2000	2000+	2000+	2000+	2000	2000+	-	2000	2000	2000	-	-	2000	2000+	-	2000	2000+	2000+	-
<i>Fridericia ulrikae</i>	2000	2000	2000+	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000+	2000
<i>Hartea perpusilla</i>	2000	0	2000	2000+	2000+	2000	2000	2000	2000	-	-	-	2000	2000+	2000+	-	2000	-	-
<i>Marionina communis</i>	2000+	2000+	2000	2000	-	750+	2000	2000	2000	-	2000	2000+	-	2000	-	0	-	-	-

Table Appendix 22: Effects of Imidacloprid on the lumbricid species for different soil layers sampling dates. – means the database is not sufficient for calculation; 2000 and 2000+: no effect could be detected; 750: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer	all	A	B	C	D	E
days after application	364	364	364	364	364	364
Aporrectodea / Allolobophora spec.	0	0	0	0	2000	2000+
Aporrectodea caliginosa	750	2000	2000	2000	2000	750+
Aporrectodea rosea	2000+	2000+	2000+	2000	2000	2000+
Lumbricus castaneus	0	0	-	-	-	-
Lumbricus rubellus	2000+	2000+	2000	2000+	-	2000
Lumbricus sp.	2000	2000	2000	2000+	2000	2000
Lumbricus terrestris	2000+	2000	-	-	750+	2000+
Octolasion cyaneum	2000	2000	2000	2000	2000+	2000
Octolasion sp.	2000	2000	2000	2000	2000	2000+

Table Appendix 23: Effects of Carbendazim on the lumbricid species for different soil layers sampling dates. – means the database is not sufficient for calculation; 15000 and 15000+: no effect could be detected; 7500: only effects for the higher concentration could be found; 0: effects for both concentrations were significant (p-value < 0.05, Williams test); +: increase in abundance

layer	all			A			B			C			D			E		
	16	114	148	16	114	148	16	114	148	16	114	148	16	114	148	16	114	148
Allolobophora chlorotica	-	-	15000	-	-	15000	-	-	-	-	-	-	-	-	-	-	-	-
Aporrectodea / Allolobophora spec.	7500	15000	0	0	0	0	15000	15000	7500	7500	15000	0	7500	15000	15000+	0+	15000	0
Aporrectodea caliginosa	15000	0	0	0	0	0	15000	0	0	15000	7500	15000	15000+	15000	15000	-	15000	15000
Aporrectodea limicola	-	-	15000	-	-	-	-	-	15000+	-	-	-	-	-	15000	-	-	15000
Aporrectodea rosea	15000	7500	0	15000	0	0	15000	7500	0	15000	0	0	-	15000	15000	-	-	15000
Lumbricus castaneus	15000	15000	0	15000	0	0	-	15000	-	-	15000	15000	-	-	-	-	-	-
Lumbricus rubellus	-	0	0	-	-	0	-	0	15000	-	15000	-	-	-	-	-	15000	-
Lumbricus sp.	0	0	0	0	0	0	0	15000	0	0	0	0	0	7500	15000	15000	0	0
Lumbricus terrestris	15000	0	0	-	-	-	-	-	-	-	-	-	15000	15000	15000	15000	0	0
Octolasion cyaneum	15000	0	0	15000	-	-	15000	-	-	15000+	0	0	0	0	0	15000+	-	15000+
Octolasion lacteum	-	-	0	-	-	-	-	-	15000	-	-	15000	-	-	15000	-	-	-
Octolasion sp.	15000	7500	15000	15000	15000	15000	15000	15000	15000	0	15000	15000	15000+	15000	15000+	-	15000	15000

3 Appendix: Additional data on the used pesticides and analytics

3.1 Physical-Chemical Property

Table Appendix 24: Physical-chemical property of Lindane. * Values for mixed isomers. Ref.: 1) Tomlin, 1996 2) Montgomery, 1993 3) Domsch, 1992

Physical-Chemical Property	Ref.	Lindane
Chemical name – IUPAC	1)	(1 <i>r</i> ,2 <i>R</i> ,3 <i>S</i> ,4 <i>r</i> ,5 <i>R</i> ,6 <i>S</i>)-1,2,3,4,5,6-hexachlorocyclohexane
Chemical name - CAS	1)	(1 <i>α</i> ,2 <i>α</i> ,3 <i>β</i> ,4 <i>α</i> ,5 <i>α</i> ,6 <i>β</i>)-gamma-hexachlorocyclohexane
CAS number	1)	58-89-9
Appearance	1)	Colourless crystals
Chemical formula	1)	C ₆ H ₆ Cl ₆
Molecular Weight	1)	290.8 g/mol
Water Solubility	1)*	0.0073 g/l (20 °C)
Solubility in Solvent	1)*	35.7 g/l in ethyl acetate (20 °C)
Melting Point	1)*	112.5 – 113.5 °C
Vapour Pressure	1) 3)	5.6 mPa (20 °C) 1.2 mPa (20 °C)
Henry´s Law Constant (H)	2)	2.0*10 ⁻¹¹ Pa m ³ /mol (23 °C)
Partition Coefficient (KOW)	2)	Log Kow = 3.2 – 3.9
Soil Adsorption Coefficient (KOC)	2)	Log Koc = 2.8 – 3.5
Stability	1)	Extremely stable to light, air, temperatures up to 180 °C and to acids.

Table Appendix 25: Physical-chemical property of Imidacloprid. Ref.: 1) Tomlin, 1996 4) Brumhard, 2004 5) Krohn, 2002 6) Canadian Water Quality Guidelines, 2007

Physical-Chemical Property	Ref.	Imidacloprid
Chemical name – IUPAC	1)	1-(6-chloro-3-pyridylmethyl)-N-nitroimidazolidin-2-ylideneamine
Chemical name - CAS	1)	1-[(6-chloro-3-pyridinyl)methyl]-N-nitro-2-imidazolidinimine
CAS number	1)	138261-41-3
Appearance	1)	Colourless crystals
Chemical formula	1)	C ₉ H ₁₀ ClN ₅ O ₂
Molecular Weight	1)	255.7 g/mol
Water Solubility	1) 5)	0.51 g/l (20 °C) 0.61 g/L (20 °C)
Solubility in Solvent	4)	50 g/l in acetonitrile
Melting Point	1)	143.8 °C
Vapour Pressure	1) 5)	0.2 µPa (20 °C) 4x 10 ⁻⁴ µPa (20 °C)
Henry´s Law Constant (H)	6)	2 * 10 ⁻¹⁰ Pa m ³ mol ⁻¹ (20 °C)
Partition Coefficient (KOW)	1)	log Kow = 0.57 (22 °C)
Soil Adsorption Coefficient (KOC)	5)	225 ml/g
Stability	1)	to hydrolysis at pH 5 - 11

Table Appendix 26: Physical-chemical property of Carbendazim. Ref. 1) EU 2010 2) ICSC 1998 3) EU 2007

Physical-Chemical Property	Ref.	Carbendazim
Chemical name – IUPAC	1)	methyl benzimidazol-2-ylcarbamate or

		2-(Methoxycarbonylamino)-benzimidazole
Chemical name - CAS	1)	methyl 1H-benzimidazol-2-ylcarbamate
CAS number	1)	10605-21-7
Appearance	1)	Light gray powder
Chemical formula	1)	C ₉ H ₉ N ₃ O ₂
Molecular Weight	1)	191.21 g/mol
Water Solubility	2)	8 mg/L
Solubility in Solvent	1)*	300mg/l (at 24 °C) in ethanol
Melting Point	2)*	302-307 °C
Vapour Pressure	3	9 x 10 ⁻⁵ Pa (20 °C); 1.5 x 10 ⁻⁴ Pa (25 °C)
Henry 's Law Constant (H)	3)	3.6 · 10 ⁻³ Pa·m ³ ·mol ⁻¹ (24 °C)
Partition Coefficient (KOW)		Log _{pow} 0.9 (pH 4); 1.5 (pH 5-9)
Soil Adsorption Coefficient (KOC)	3	200 - 246
Stability		Hydrolytic stability pH 5: > 350 d (22 °C)

3.2 Results of Preliminary-screening simulations with PELMO

3.2.1 Input data selection

Simulations were performed with PELMO 4.4.3 in order to find optimum conditions for the experiments in this project. For these initial simulations the following input parameters were used.

Table Appendix 27: Input parameters of the active compounds for the PELMO-Pre-screening Simulations

	Imidacloprid	Lindan
KOC (L/kg)	223	1200
Freundlich	0.8	0.9
DT50	103.8	260
Q10	2.58	2.58
Walker	0.7	0.7
Vapour pressure (Pa)	0	0.01
Wasser solubility (mg/L)	0	7.0
Application rate (kg/ha)	2	75

The following soil input data on organic carbon content and pH, which belong to the used soil cores during the experiment, were considered for the pre-screening simulations. As the soil cores were only 25 cm deep biodegradation was not reduced with depth (biodegradation factor =1).

Table Appendix 28: Available properties of the experimental soils

Layer	Corg (%)	pH	Biodegradation factor
0 - 5 cm	4.7	6.5	1
5 - 10 cm	3.1	6.1	1
10 - 25 cm	2.7	6.2	1

As for modelling with PELMO the available soil information was not sufficient the remaining input parameters were estimated as shown in the following table. The initial soil moisture was set to 30 Vol%.

Table Appendix 29: Additional assumptions for the experimental soil profile

Layer	Sand content	Silt content	Clay content	Theta FC	Theta WP	Disp.
	(%)	(%)	(%)	(m3.m-3)	(m3.m-3)	(cm)
0 - 5 cm	16.2	39.2	44.6	0.4482	0.2776	2.5
5 - 10 cm	16.5	37.9	45.6	0.4395	0.2961	2.5
10 - 25 cm	16.1	38.4	45.5	0.4395	0.2961	2.5

In order to ensure maximum transport of the compounds a relatively wet climate was selected which was based on the FOCUS scenario Okehampton with annual precipitation of about 1040 mm. Finally, all simulations were performed considering the FOCUS crop "Grass/alfalfa" with application on the 1st May.

3.2.2 Results

3.2.2.1 Leachate

Simulations were performed over 4 years. The following figure shows the daily cumulative leachate compared to the cumulative precipitation.

The amount of leachate rather than the precipitation is most important for the transport of the active substances in deeper soil layers over time depending of their fate and adsorption properties.

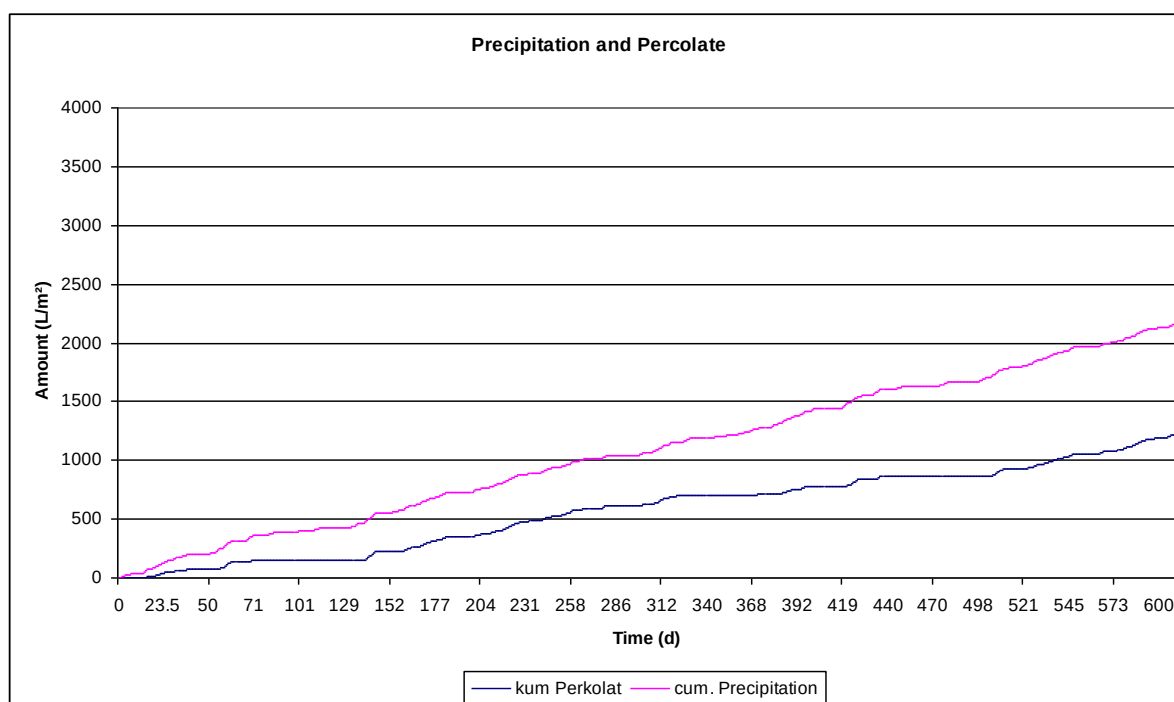


Figure appendix 1: Cumulative precipitation and leachate amount in the pre-screening simulations with PELMO (Okehampton scenario)

3.2.2.2 Lindane

Simulations were performed over 4 years. Due to the variability of sorption and degradation of lindane in different soils the uncertainty of the exposure simulation of lindane was rather high.

Figure A31 shows the calculated lindane concentration in soil in the top 5 cm together with the cumulative precipitation amount. The maximum concentration of 120 mg/kg is reduced by 50% after one year caused by degradation and some leaching.

Figure A32 shows calculated lindane concentrations at 5 – 10 cm. They show maximum concentrations after about two years (3500 mm precipitation and 2000 mm leachate). Due to the dispersion in soil the increase of concentrations is already beginning in the first winter.

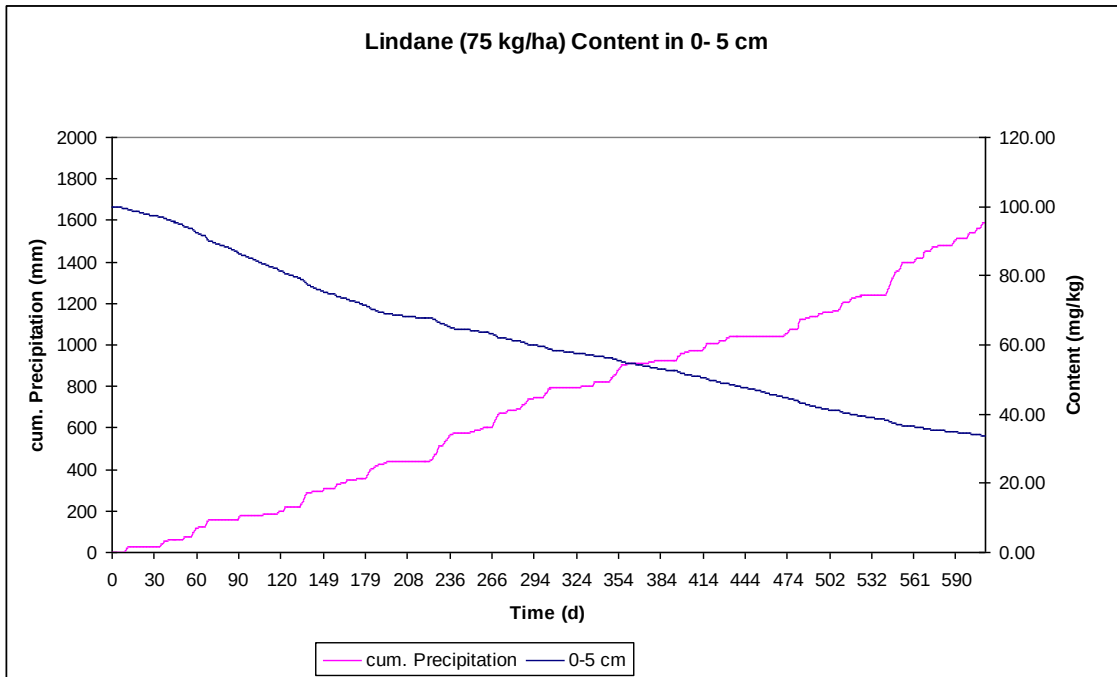


Figure appendix 2: Cumulative precipitation and lindane concentration in the top 5 cm soil (pre-screening simulations with PELMO for Okehampton)

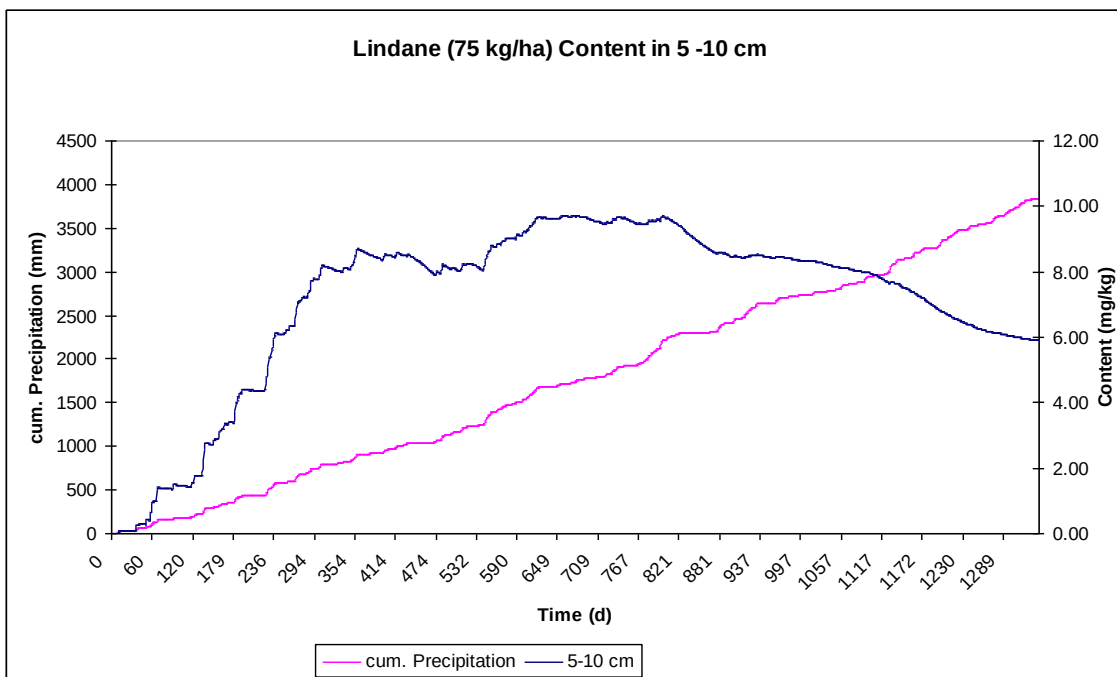


Figure appendix 3: Cumulative precipitation and lindane concentration in the top 5 - 10 cm soil (pre-screening simulations with PELMO for Okehampton)

As shown by the following figure the simulation predicts a slow increase of the concentrations that starts already in the first winter. Even after 4 years the maximum in the 10-15 cm soil layer is not reached. The calculated maximum concentrations are about two orders of magnitude below the maximum concentrations in the top soil layer.

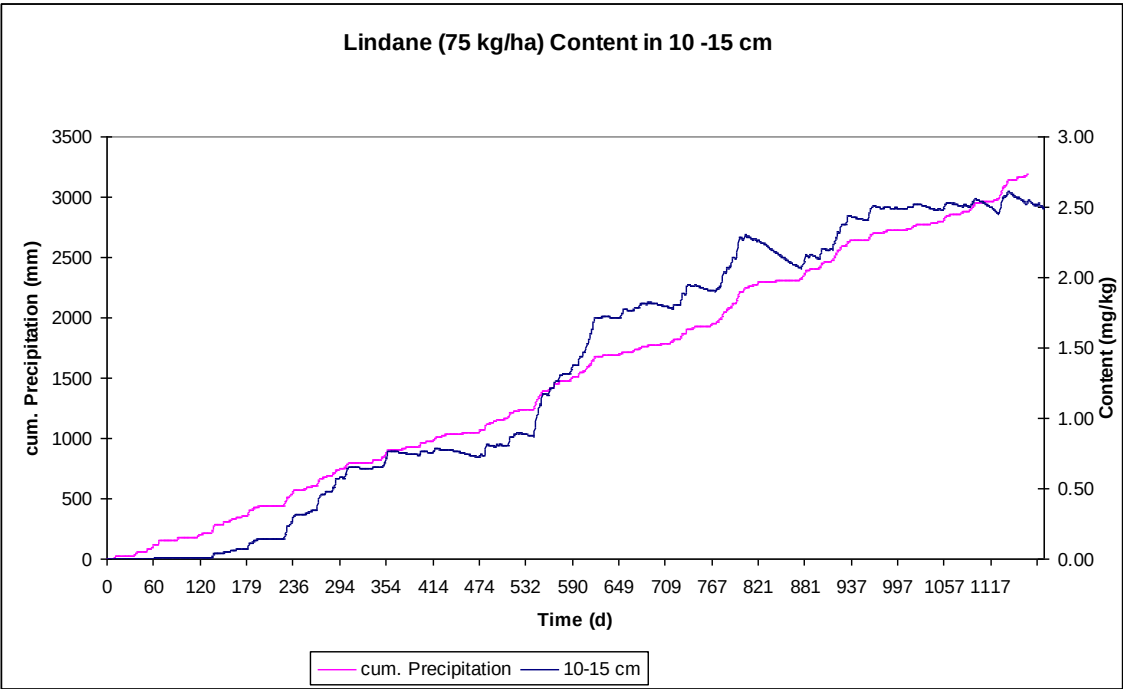


Figure appendix 4: Cumulative precipitation and lindane concentration at the top 10 - 15 cm soil (pre-screening simulations with PELMO for Okehampton)

The final figure presents results for the 15-20 cm soil layer. The concentrations remain below 1 mg/kg even after four years. The concentrations in soil exceeds 0.2 mg/kg after about 2 years and more than 1000 mm leachate.

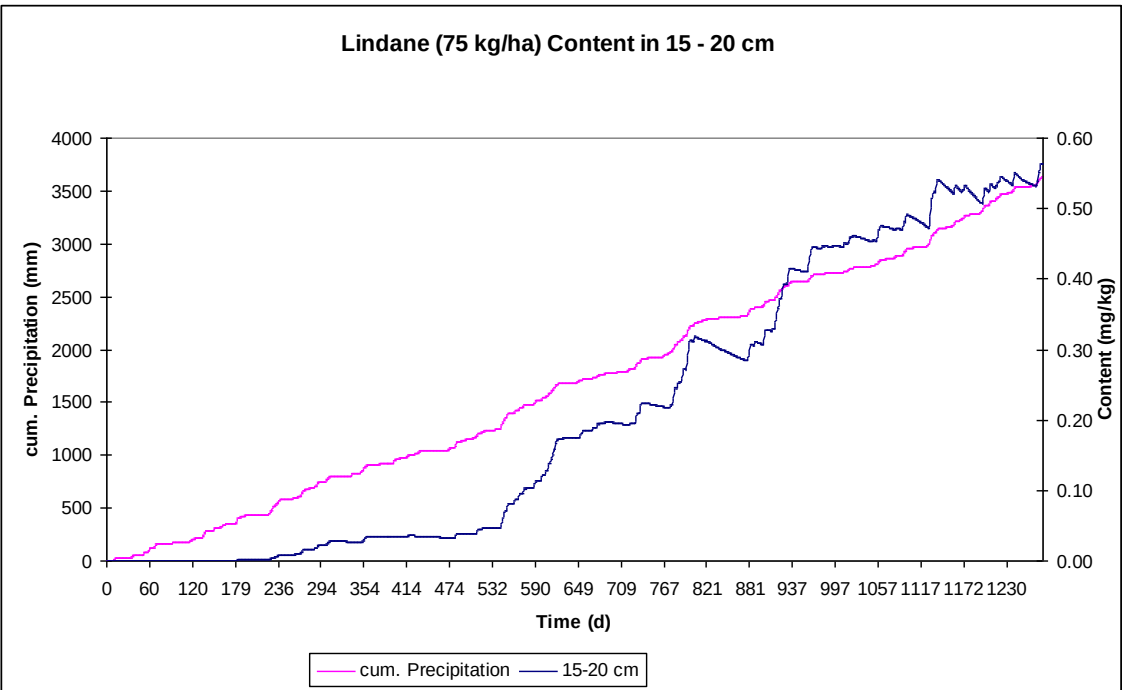


Figure appendix 5: Cumulative precipitation and lindane concentration at the top 15 - 20 cm soil (pre-screening simulations with PELMO for Okehampton)

Summarizing results including a graphical presentation of the calculated lindane concentration in the soil 14 days and 180 days after application is given in chapter 3.3.1 of the report.

3.2.2.3 Imidacloprid

In the following figure the calculated soil concentrations are presented for imidacloprid. The maximum concentration of 2.7 mg/kg is reduced by 50% within 135 days due to leaching and degradation.

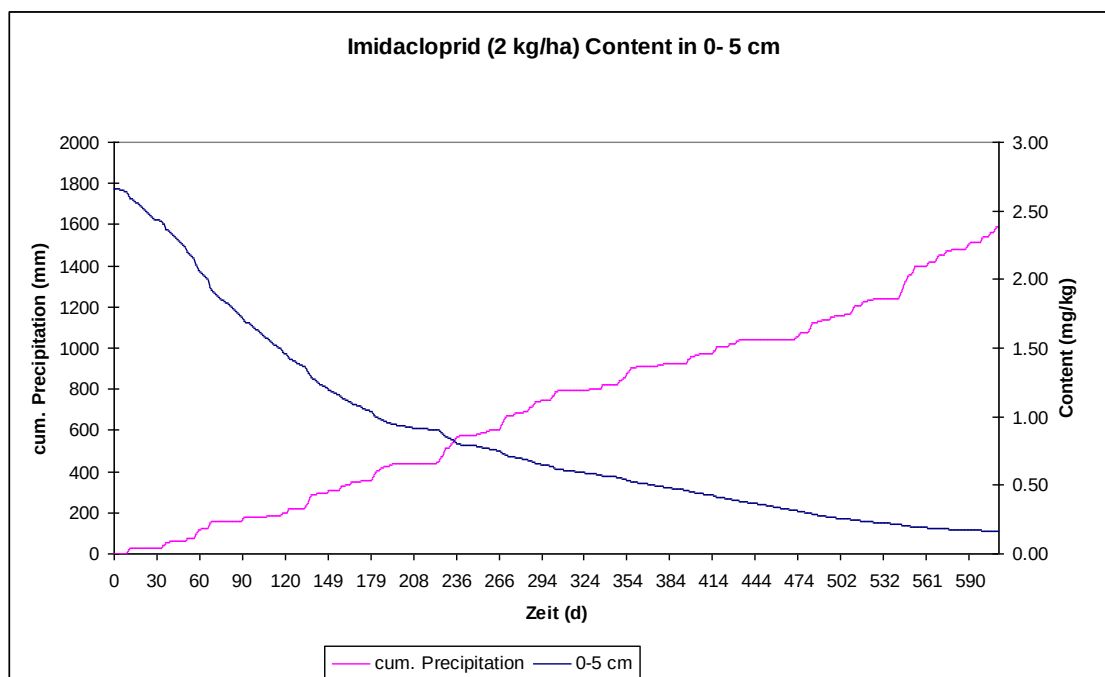


Figure appendix 6: Cumulative precipitation and imidacloprid concentration at the top 0-5 cm soil (pre-screening simulations with PELMO for Okehampton)

Figure A3_7 shows calculated soil concentrations at 5-10 cm. In this soil layer, the maximum concentration is reached after about 300 days (and 400 mm leachate).

In figure A3_8 the daily concentrations are presented for the 10-15 cm soil layer. The maximum concentration is reached already after 1 year (about 450 mm leachate). In the following autumn the imidacloprid concentration is increasing again.

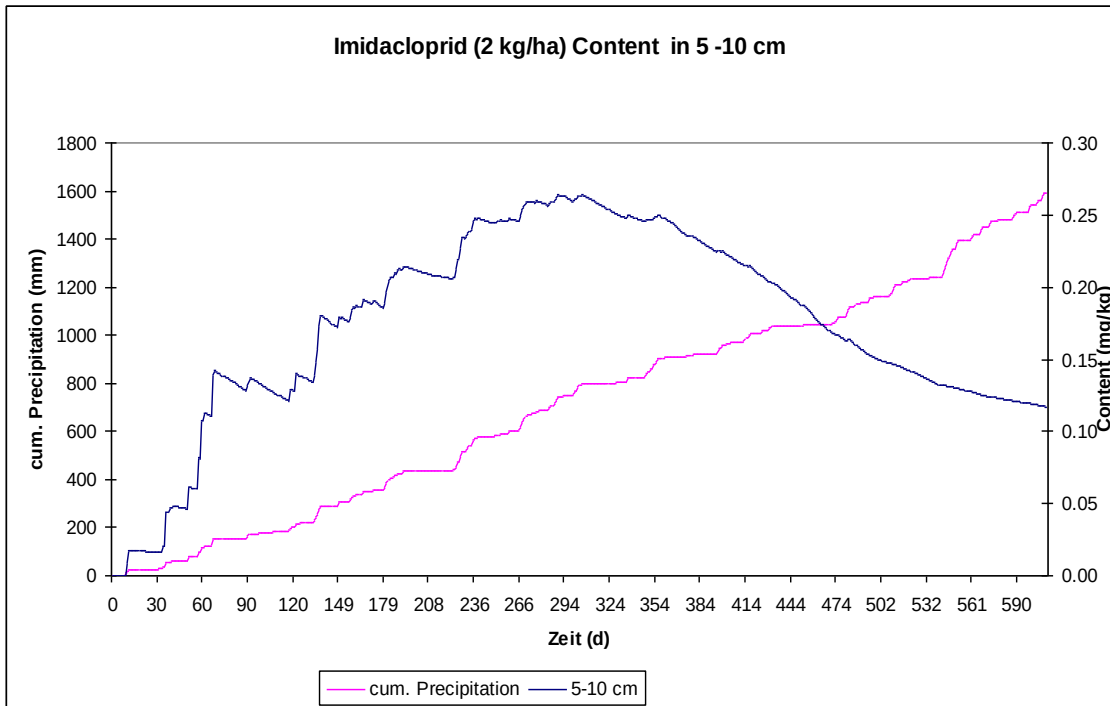


Figure appendix 7: Cumulative precipitation and imidacloprid concentration at the top 5-10 cm soil (pre-screening simulations with PELMO for Okehampton)

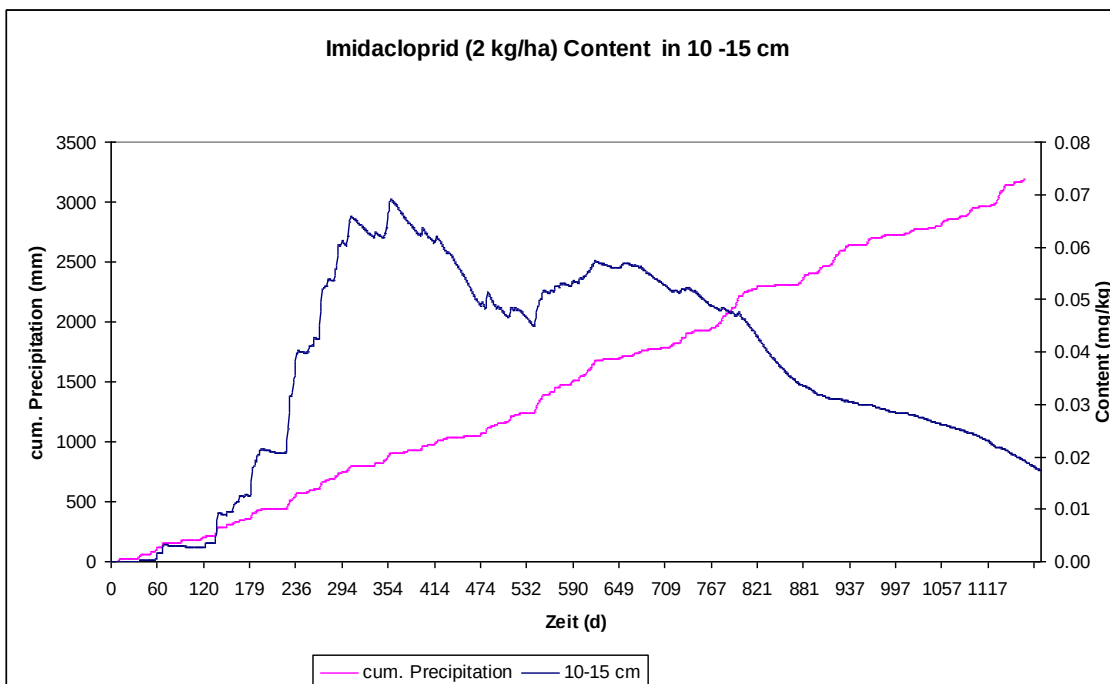


Figure appendix 8: Cumulative precipitation and imidacloprid concentration at the top 10-15 cm soil (pre-screening simulations with PELMO for Okehampton)

The final figure shows the situation at 15-20 soil depth. Here, the maximum concentration is reached after 800 days (1000 mm leachate). However, the concentrations are rather low.

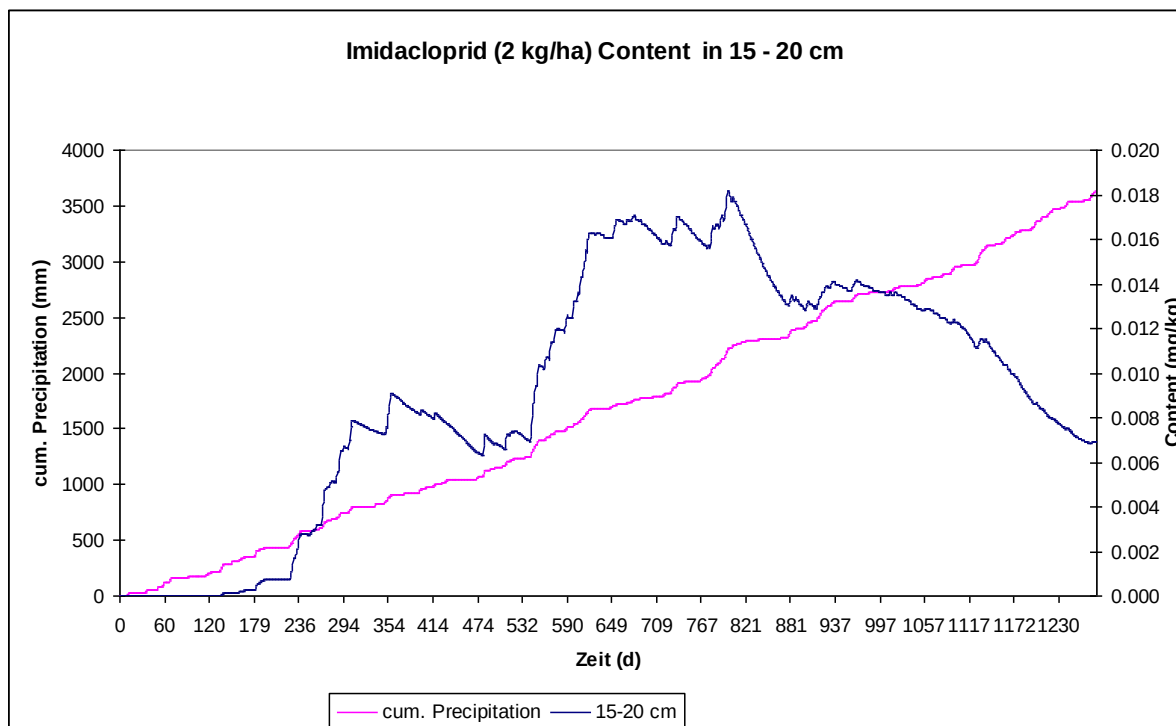


Figure appendix 9: Cumulative precipitation and imidacloprid concentration at the top 15-20 cm (pre-screening simulations with PELMO for Okehampton)

Summarizing results including a graphical presentation of the calculated imidacloprid concentration in the soil 14 days and 180 days after application is given in chapter 3.3.1 of the report.

3.3 Parameters for LC-MS/MS

Table Appendix 30: Liquid Chromatographic Conditions:

Column: Hypersil Gold PFP, Length 150 mm, i.d. 4.0 mm, Particle Size 3 µm, Part No 25403-154030, Thermo Fisher Scientific, 58239 Schwerte, Germany

Injection volume: 10 µl, Oven temperature: Ambient, 20 °C

Mobile phases: A: water / formic acid (99,5/0,5; v/v)
 B: acetonitrile / formic acid (99,5/0,5; v/v)

Run time: 28 min

Flow rate: 0,4 ml / min

Retention times: Imidacloprid and d4-Imidacloprid: approx. 5 min

Table Appendix 31: HPLC Gradient

Time [min]	0	10	12	15	17	28
% A (water / formic acid; 99.5/0.5; v/v)	10	10	90	90	10	10
% B (acetonitril / formic acid; 99.5/0.5; v/v)	90	90	10	10	90	90

Table Appendix 32: Parameter der Electro-Spray-Ionisierung:

Parameters with positive Ionisation:	
Source Type	HESI
Capillary Temperature	275 °C
Vaporizer Temperature	75 °C
Sheath Gas Flow	40
Aux Gas Flow	15
Sweep Gas Flow	0
Source Voltage	4 kV
Source Current	100 µA
Capillary Voltage	21 V
Tube Lens	65 V

Table Appendix 33: MS/MS- Parameter

Acquire time	28 min
Mass Resolution	30000
Polarity	Positive
Scan Event 1	FTMS + c Full ms [100-500 m/z], res=30000, CV = 0.0 V
Scan Event 2	FTMS + c norm x (256.00)->[70.0-300.0], res = 15000 MS/MS with the parent mass (m/z): 256 Act. Type: CID, Iso. Width (m/z): 1.0, Act. Q: 0,250 Normalized Collision Energy: 35,0, SID = 35.0 V, CV = 0.0 V Act. Time (ms): 30.0

3.4 Method of Combustion

After extraction of the soil or vegetation, the remaining samples were homogenized and aliquots of about 2 g were removed and kept in an desiccator (Lindane samples) or dry cabinet (Imidacloprid samples) overnight. Then aliquots of about 0.4 g soil or 0.25 g vegetation were weight into combustion cones.

The soil or vegetation samples were filled into combustion-cones, which were inserted into the oxidizer and combusted in an oxygen atmosphere at a high temperature for 4 min.

In Table Appendix 34 the parameters of the combustion procedure are summarized. During this procedure, organic compounds are combusted to $^{14}\text{CO}_2$ or CO_2 and H_2O using a catalyst.

The CO_2 formed were trapped using 16 ml of scintillator. The apparatus was cleaned by an N_2 stream after each combustion cycle. The samples were examined by liquid scintillation counting.

Table Appendix 34: Parameter used with the Biological Oxidizer OX501

N ₂ stream	325 ml/min
O ₂ stream	325 ml/min
Combustion temperature	900°C
Catalyst temperature	680°C
Combustion cycle	4 min (samples); 2 min (references)

Prior to the combustion of the samples from the experiments, the oxidation efficiency was examined:

- 3 combustions cycles without introduction of any material (E): were performed to clean the system.
- 3 combustions of an oxidizer cap each (B): These served as blank combustions.
- 3 standards (ST): 10 µl of standard solution were directly applied into a scintillation vial. It contained about 8000 dpm. Combustion occurred without introduction of any material.
- 3 combustions of the standard (STC): Ca. 100 mg of cellulose (Merck) and 10 µl of the standard solution were placed in a cellulose cap and combusted. After 10 combustions each, one standard was additionally combusted to control the performance of the apparatus.

For each, the T, ST and STC combustions a mean value was determined. These mean values were inserted into the following equation to calculate the correction factor (F):

3.5 Analyses of Lindane, calibration and recovery in water

Table Appendix 35: Standard L8 (308,7 ng/ml) in ethyl acetate (Std_L8_E) and matrix (Std_L8_M), respectively. Three injections of one vial.

Solution	Area	Mean $\pm$ SD
Std_L8_E-1	16602519	16,874,261 $\pm$ 272,489
Std_L8_E-2	16872774	
Std_L8_E-3	17147491	
Std_L8_M-1	15692387	15,740,273 $\pm$ 41,573
Std_L8_M-2	15767125	
Std_L8_M-3	15761308	

Table Appendix 36: Three parallel extracts (3a,3b,3c) from soil 3 (42,949 g Na₂SO₄-soil mixture spiked with 154,35 μ g Lindane).

The mean of two injections from each vial is shown. Calculated results while using standards in ethyl acetate and in matrix

Solution	Area mean $\pm$ SD	in ethyl acetate		in matrix	
		ug/kg soil	Recovery	ug/kg soil	Recovery
Soil_3a	19,482,941 $\pm$ 235,448	2832	78,8%	3036	84,5%
Soil_3b	19,010,347 $\pm$ 200,046	2721	75,7%	2917	81,2%
Soil_3c	18,775,964 $\pm$ 104,392	2658	74,0%	2850	79,3%
mean of all:	19,089,751 $\pm$ 353,577	2736	76,1%	2934	81,6%

Table Appendix 37: Recovery of Lindane in 100 ml of spiked water (a, b, and c refer to replicate analyses).

Sample	Recovery (%)	Sample	Recovery (%)
1 μ g -a	91.2	10 μ g	96.7
	90.2		97.1
1 μ g -b	87.4		
	88.6		
1 μ g -c	91.4		
	92.4		
Mean	90.2 $\pm$ 1.9	Mean	96.9 $\pm$ 0.3

3.6 Analyses of Imidacloprid, calibration and recovery in water

Table Appendix 38: Results of the measurement of calibration solutions of Imidacloprid.

m/z Area Imi 256.055 - 256.065	m/z Area IS 260.080 - 260.090	Ratio Imi/IS	Conz ng/ml
712,125	2,331,846	0.31	49
1,187,076	2,369,185	0.50	78.4
1,555,734	2,412,118	0.64	98
2,328,389	2,388,287	0.97	147
3,006,441	2,173,720	1.38	196
2,856,442	1,678,434	1.70	245
4,804,861	2,314,689	2.08	294
6,206,002	2,262,991	2.74	392
7,987,826	2,347,783	3.40	490
9,509,992	2,268,824	4.19	588

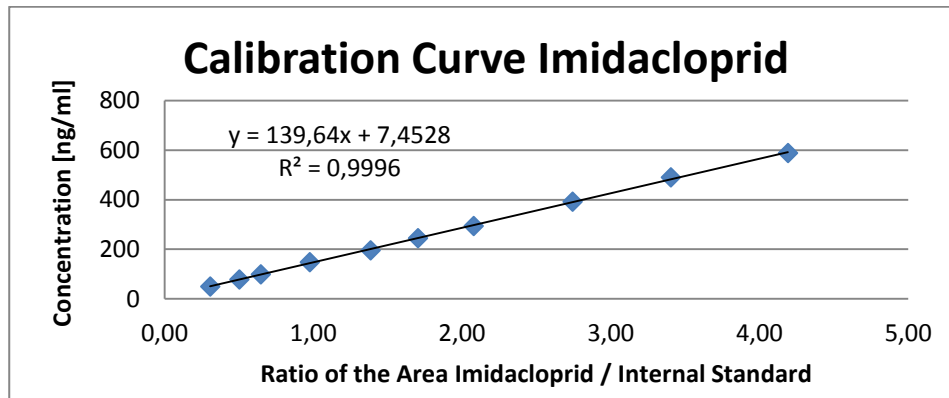


Figure appendix 10: Calibration curve for the measurement of Imidacloprid samples.

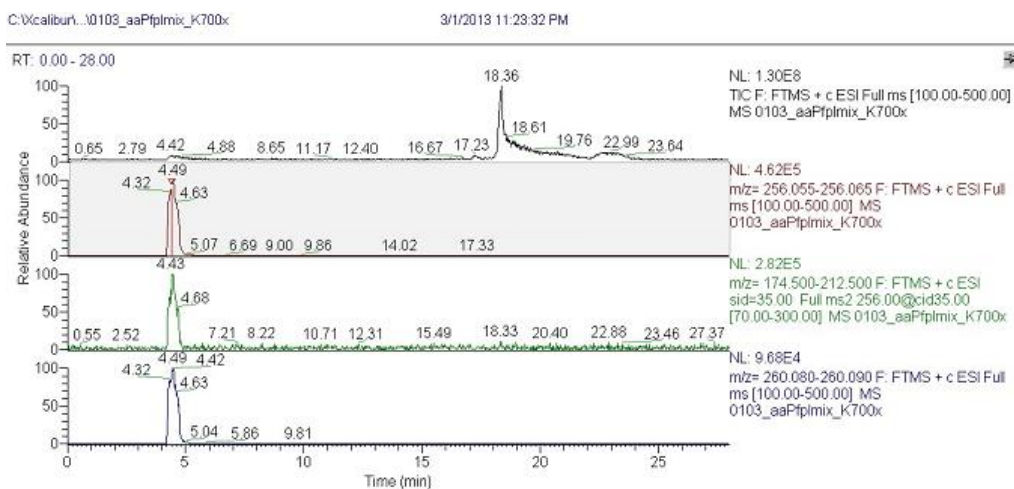


Figure appendix 11: Chromatogram of an extract with Imidacloprid. Shown are the total ion chromatogram (black), the selected ion chromatogram of Imidacloprid (m/z 256.055-256.065, red), the MS/MS-chromatogram of the mass 256.0 (m/z 174.5 – 212.5, green) and the selected ion chromatogram of d4-Imidacloprid (m/z 260.08 – 260.09, blue)

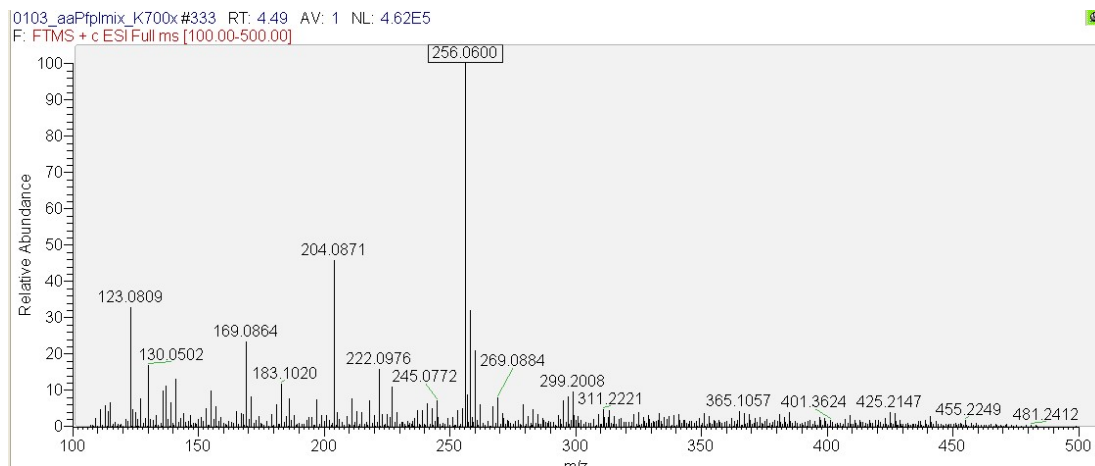


Figure appendix 12: MS-spectrum of minute 4.49. The mass 256.0600 correspond to Imidacloprid.

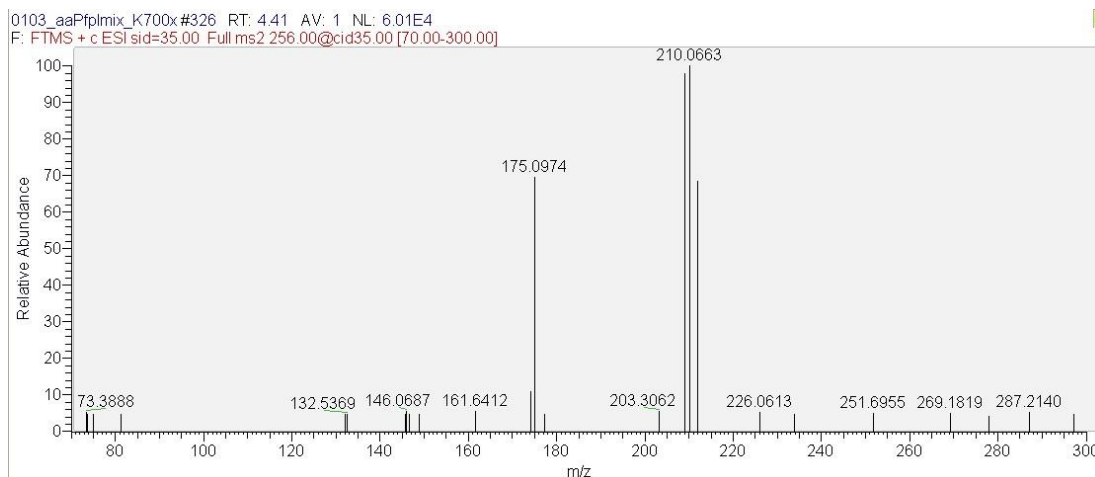


Figure appendix 13: MS/MS-spectrum of m/z 265.0 at minute 4.41. The masses 175, 209, 210 and 212 are known fragments of Imidacloprid.

Table Appendix 39: Recovery of Imidacloprid in water from calibration solutions

Sample	Recovery (%)	Sample	Recovery (%)
19.61 µg/L	103.78	49.00 µg/L	93.39
	100.86		104.68
29.40 µg/L	91.65	78.40 µg/L	104.42
	86.60		101.65
Mean ± SD	98.38 ± 6.88		

3.7 Weight of Samples and Content of Dry Matter

Table Appendix 40: Field study: Soil weight and dry matter content of (unlabeled) Lindane samples. Measured are the content of dry matter in control samples after sampling.

	Application of 7.5 kg/ha	Application of 20 kg/ha	
	Soil weight [g] ± SD	Soil weight [g] ± SD	Soil dry matter content [%]
Sampling T0, 1 day after application			
Layer A: 0 - 2.5 cm	45.1 ± 7.0	44.9 ± 9.7	64.8 ± 1.2
Layer B: 2.5 - 5 cm	56.9 ± 10.9	44.3 ± 10.9	76.3 ± 1.4
Layer C: 5 - 10 cm	109.6	110.2	80.5 ± 3.8
Sampling T1, 14 days after application			
Layer A: 0 - 2.5 cm	42.9 ± 10.1	40.2 ± 4.9	68.0 ± 2.9
Layer B: 2.5 - 5 cm	36.6 ± 13.8	41.6 ± 10.6	74.6 ± 5.1
Layer C: 5 - 10 cm	114.3 ± 31.4	107.5 ± 26.2	80.6 ± 3.4
Layer D: 10 - 20 cm	-	222.8 ± 40.3	-
Sampling T2, 42 days after application			
Layer A: 0 - 2.5 cm	53.3 ± 4.3	59.7 ± 6.7	57.2 ± 0.2
Layer B: 2.5 - 5 cm	61.4 ± 6.6	55.8 ± 10.1	68.2 ± 2.3
Layer C: 5 - 10 cm	115.2 ± 50.7	106.4 ± 8.6	74.8 ± 2.3
Layer D: 10 - 20 cm	166	159.3	-
Sampling T3, 140 days after application			
Layer A: 0 - 2.5 cm	44.7 ± 8.8	41.7 ± 6.3	69.5 ± 5.2
Layer B: 2.5 - 5 cm	42.3 ± 6.5	46.6 ± 7.0	72.8 ± 3.6
Layer C: 5 - 10 cm	110.5 ± 28.5	115.6 ± 43.5	76.0 ± 0.9
Layer D: 10 - 20 cm	228.9 ± 13.5	163.9 ± 32.3	-
Sampling T4, 189 days after application			
Layer A: 0 - 2.5 cm	40.8 ± 9.6	44.5 ± 7.7	59.5 ± 1.0
Layer B: 2.5 - 5 cm	48.8 ± 12.7	46.3 ± 7.6	66.7 ± 1.3
Layer C: 5 - 10 cm	128.3 ± 23.1	110.3 ± 13.1	72.0 ± 1.9
Layer D: 10 - 20 cm	147.6 ± 3.5	155.5 ± 13.2	-
Sampling T5, 365 days after application			
Layer A: 0 - 2.5 cm	37.8 ± 10.1	40.5 ± 4.9	56.6 ± 2.1
Layer B: 2.5 - 5 cm	47.7 ± 11.8	50.7 ± 12.7	61.8 ± 2.3
Layer C: 5 - 10 cm	113.3 ± 18.9	117.2 ± 5.6	70.8 ± 3.7
Layer D: 10 - 20 cm	146.8 ± 17.8	159.0 ± 10.2	-

Table Appendix 41: Field study: Soil weight and dry matter content of (unlabeled) Imidacloprid samples. Measured are the contents of dry matter in analysed samples prior to analyses.

	Application of 0,75 kg/ha	Application of 2 kg/ha	
	Soil weight [g] ± SD	Soil weight [g] ± SD	Soil dry matter content [%]
Sampling T0, 1 day after application			
Layer A: 0 - 2.5 cm	47.0 ± 5.8	45.3 ± 3.6	68.4 ± 3.4
Layer B: 2.5 - 5 cm	50.0 ± 9.3	47.9 ± 10.2	75.7 ± 5.8
Layer C: 5 - 10 cm	110.153	100.939	82.0 ± 0.3
Sampling T1, 14 days after application			
Layer A: 0 - 2.5 cm	42.8 ± 7.2	39.9 ± 1.6	68.4 ± 5.1
Layer B: 2.5 - 5 cm	47.4 ± 8.1	33.4 ± 6.5	76.7 ± 2.9
Layer C: 5 - 10 cm	110.1 ± 12.6	112.5 ± 18.0	80.9 ± 1.3
Layer D: 10 - 20 cm	221.9 ± 17.4	225.9 ± 50.3	79.5 ± 2.1
Sampling T2, 42 days after application			
Layer A: 0 - 2.5 cm	52.9 ± 8.1	49.2 ± 6.5	58.3 ± 4.3
Layer B: 2.5 - 5 cm	51.1 ± 11.0	49.4 ± 7.6	66.4 ± 4.8
Layer C: 5 - 10 cm	131.0 ± 12.5	140.9 ± 2.8	72.5 ± 3.6
Layer D: 10 - 20 cm	251.4 ± 18.8	281.2 ± 35.1	73.9 ± 1.3
Sampling T3, 140 days after application			
Layer A: 0 - 2.5 cm	48.8 ± 4.3	46.9 ± 9.5	66.6 ± 5.0
Layer B: 2.5 - 5 cm	48.4 ± 6.2	45.4 ± 14.1	71.0 ± 5.2
Layer C: 5 - 10 cm	148.0 ± 4.6	129.1 ± 6.4	75.5 ± 1.9
Layer D: 10 - 20 cm	205.2 ± 34.0	253.7 ± 17.2	75.9 ± 1.5
Sampling T4, 189 days after application			
Layer A: 0 - 2.5 cm	31.9 ± 1.5	36.6 ± 3.9	59.2 ± 4.0
Layer B: 2.5 - 5 cm	64.7 ± 5.8	51.8 ± 10.1	66.5 ± 1.8
Layer C: 5 - 10 cm	125.9 ± 1.3	130.3 ± 4.7	73.3 ± 2.0
Layer D: 10 - 20 cm	200.1 ± 11.4	205.2 ± 2.4	73.2 ± 1.5
Sampling T5, 365 days after application			
Layer A: 0 - 2.5 cm	46.8 ± 4.7	42.9 ± 4.7	56.2 ± 2.8
Layer B: 2.5 - 5 cm	47.2 ± 5.4	48.1 ± 5.9	61.7 ± 3.5
Layer C: 5 - 10 cm	101.6 ± 6.2	121.6 ± 16.1	69.6 ± 2.5
Layer D: 10 - 20 cm	205.9 ± 32.9	244.2 ± 11.5	70.6 ± 1.5

Table Appendix 42: Laboratory study: Soil weight and dry matter content of (¹⁴C-labeled) Lindane samples. *) supposed weight of sample.

	Application of 2 kg/ha	
	Soil weight [g]	Soil dry matter content [%]
Sampling T0, 1 day after application		
Layer A1: 0 - 1 cm	96.3	53.3
Layer A2: 1 – 2.5 cm	183.1	59.8 ± 1.9
Layer B: 2.5 - 5 cm	282.6	72.8 ± 2.8
Layer C: 5 - 10 cm		73.5 ± 3.4
Layer D: 10 - 20 cm		76.9 ± 0.7
Sampling T1, 14 days after application		
Layer A1: 0 - 1 cm	83.2	51.9
Layer A2: 1 – 2.5 cm	210.8	56.2 ± 3.8
Layer B: 2.5 - 5 cm	382.9	65.7 ± 1.9
Layer C: 5 - 10 cm	650*	72.8 ± 1.8
Layer D: 10 - 20 cm		74.9 ± 2.9
Sampling T2, 42 days after application		
Layer A1: 0 - 1 cm	124.3	45.7
Layer A2: 1 – 2.5 cm	277.6	53.7 ± 6.6
Layer B: 2.5 - 5 cm	299.5	62.7 ± 1.0
Layer C: 5 - 10 cm	650*	68.4 ± 2.1
Layer D: 10 - 20 cm	1543.9	72.8 ± 0.4
Sampling T3, 140 days after application		
Layer A1: 0 - 1 cm	41.1	62.1
Layer A2: 1 – 2.5 cm	114.2	70.5 ± 1.0
Layer B: 2.5 - 5 cm	270.9	76.5 ± 1.4
Layer C: 5 - 10 cm	639.7	79.8 ± 1.3
Layer D: 10 - 20 cm	1475.9	82.2 ± 2.8
Sampling T4, 189 days after application		
Layer A1: 0 - 1 cm	43.3	76.9
Layer A2: 1 – 2.5 cm	116.2	68.3 ± 1.3
Layer B: 2.5 - 5 cm	230.3	77.9 ± 1.2
Layer C: 5 - 10 cm	682.0	77.8 ± 0.4
Layer D: 10 - 20 cm	1507.3	76.6 ± 1.1

Table Appendix 43: Laboratory study: Soil weight and dry matter content of (¹⁴C-labeled) Imidacloprid samples. *) supposed weight of sample.

	Application of 2 kg/ha	
	Soil weight [g]	Soil dry matter content [%]
Sampling T0, 1 day after application		
Layer A1: 0 - 1 cm	90.3	56.1
Layer A2: 1 – 2.5 cm	197.6	67.1 ± 1.4
Layer B: 2.5 - 5 cm	202.2	73.0 ± 0.2
Layer C: 5 - 10 cm		80.6 ± 4.4
Layer D: 10 - 20 cm		77.7 ± 3.8
Sampling T1, 14 days after application		
Layer A1: 0 - 1 cm	42.4	69.3
Layer A2: 1 – 2.5 cm	162.8	69.8 ± 2.3
Layer B: 2.5 - 5 cm	287.8	76.1 ± 0.5
Layer C: 5 - 10 cm	700*	78.0 ± 0.1
Layer D: 10 - 20 cm	1400*	77.4 ± 1.2
Sampling T2, 42 days after application		
Layer A1: 0 - 1 cm	124.8	50.5
Layer A2: 1 – 2.5 cm	184.1	44.7 ± 6.3
Layer B: 2.5 - 5 cm	269.9	57.8 ± 0.2
Layer C: 5 - 10 cm	747.2	71.7 ± 1.8
Layer D: 10 - 20 cm	1426.1	71.9 ± 1.3
Sampling T3, 140 days after application		
Layer A1: 0 - 1 cm	60.5	71.3 ± 0.2
Layer A2: 1 – 2.5 cm	110.6	69.6 ± 0.9
Layer B: 2.5 - 5 cm	329.2	74.8 ± 3.0
Layer C: 5 - 10 cm	634.4	82.4 ± 0.7
Layer D: 10 - 20 cm	1670.1	80.3 ± 1.2
Sampling T4, 189 days after application		
Layer A1: 0 - 1 cm	48.1	77.9 ± 0.9
Layer A2: 1 – 2.5 cm	115.0	65.5 ± 0.9
Layer B: 2.5 - 5 cm	257.9	78.3 ± 2.6
Layer C: 5 - 10 cm	676.4	76.6 ± 1.6
Layer D: 10 - 20 cm	1448.0	78.0 ± 3.9

3.8 Concentration of Lindane and Imidacloprid in soil (field study)

Table appendix 44: Concentration (Conc.) of Lindane in soil $\pm$ standard derivation. Not detectable = n.d., below the limit of quantification = < LOQ, n.a. = not analysed. The median of two values is equal to the mean, so it is not shown.

Application of 0,75 kg/ha of Lindane				Application of 20 kg/ha of Lindane			
TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core	TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core
T0: 1 day after application							
Layer A: 0 – 2.5 cm depth							
10	L10Aa	23.03 ± 1.32	683.24	31	L20Aa	83.77 ± 14.5	1990.91
28	L10Ac	27.80 ± 2.23	713.80	41	L20Ac	59.39 ± 4.07	1776.53
26	L10Ad	74.43 ± 5.05	1970.40	29	L20Ad	57.07 ± 5.41	2013.54
45	L10Ae	12.95 ± 0.58	358.77	38	L20Ae	45.71 ± 0.76	1531.45
16	L10Af	18.57 ± 1.77	705.17	18	L20Af	27.89 ± 1.21	915.57
42	L10Ag	13.65 ± 0.39	378.16	22	L20Ag	95.31 ± 1.22	1833.39
mean = 28.41 ± 23.24 median = 20.80				mean = 61.52 ± 24.67 median = 58.23			
Layer B: 2.5 – 5 cm depth							
10	L10Ba	0.285 ± 0.042	15.39	31	L20Ba	0.017 ± 0.001	0.55
28	L10Bc	0.128 ± 0.002	5.40	41	L20Bc	0.030 ± 0.001	0.90
26	L10Bd	0.528 ± 0.015	27.34	29	L20Bd	0.149 ± 0.023	4.07
45	L10Be	< 0,015	0.31	38	L20Be	0.673 ± 0.004	33.79
16	L10Bf	0.870 ± 0.077	37.05	18	L20Bf	0.045 ± 0.001	1.51
42	L10Bg	0.032 ± 0.003	1.01	22	L20Bg	0.026 ± 0.003	0.76
mean = 0.309 ± 0.336 median = 0.207				mean = 0.157 ± 0.258 median = 0.037			
Layer C: 5 – 10 cm depth							
10	L10Ca	< 0,015	0.71	31	L20Ca	< 0,014	0.62
T1: 14 days after application							
Layer A: 0 – 2.5 cm depth							
10	L11Aa	37.65 ± 4.13	829.10	31	L21Aa	66.15 ± 9.90	1637.01
10	L11Ab	15.00 ± 0.17	445.32	31	L21Ab	80.43 ± 5.10	1973.56
28	L11Ac	18.42 ± 1.57	438.10	41	L21Ac	49.60 ± 8.85	1269.51
26	L11Ad	7.11 ± 0.53	169.83	29	L21Ad	33.06 ± 3.01	856.64
45	L11Ae	15.94 ± 2.25	490.56	38	L21Ae	22.78 ± 2.65	733.31
16	L11Af	32.99 ± 3.36	1043.45	18	L21Af	32.42 ± 4.72	998.67
42	L11Ag	17.25 ± 0.62	725.08	22	L21 g	24.27 ± 2.50 ¹⁾	1470.20
mean = 20.62 ± 10.76 median = 17.25				mean = 47.41 ± 22.29 median = 41.33			
Layer B: 2.5 – 5 cm depth							
10	L11Ba	2.035 ± 0.161	32.20	31	L21Ba	0.693 ± 0.085	13.71
10	L11Bb	0.118 ± 0.009	1.85	31	L21Bb	1.686 ± 0.063	65.95
28	L11Bc	0.338 ± 0.053	7.90	41	L21Bc	0.147 ± 0.004	5.25
26	L11Bd	<0,023	0.42	29	L21Bd	0.108 ± 0.006	3.04
45	L11Be	0.336 ± 0.005	7.88	38	L21Be	0.158 ± 0.016	6.06
16	L11Bf	0.020 ± 0.003	0.69	18	L21Bf	0.086 ± 0.011	2.17
42	L11Bg	0.861 ± 0.078	34.57	22	¹⁾ analysed with Layer A		
mean = 0.531 ± 0.724 median = 0.336				mean = 0.480 ± 0.634 median = 0.152			
Lindane, continued							
TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core	TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core
Layer C: 5 – 10 cm depth							
10	L11Ca	0.229 ± 0.026	25.20	31	L21Ca	0.140 ± 0.027	8.93

10	L11Cb	0.033 ± 0.002	4.19	31	L21Cb	0.500 ± 0.093	48.17
28	L11Cc	0.141 ± 0.001	15.63	41	L21Cc	0.172 ± 0.015	16.67
26	L11Cd	0.024 ± 0.001	1.54	29	L21Cd	0.108 ± 0.006	10.32
45	L11Ce	0.341 ± 0.008	26.61	38	L21Ce	0.252 ± 0.058	23.10
16	L11Cf	0.137 ± 0.002	8.05	18	L21Cf	0.573 ± 0.084	29.30
42	L11Cg	0.112 ± 0.004	10.68	22	L21Cg	0.572 ± 0.053	63.35
mean = 0.145 ± 0.111 median = 0.137				mean = 0.331 ± 0.209 median = 0.212			
Layer D: 10 – 20 cm depth							
	n.a.			31	L214a	0.106 ± 0.001	21.37
				31	L214b	0.063 ± 0.001	9.79
				mean = 0.084 ± 0.030			
T2: 42 days after application							
Layer A: 0 – 2.5 cm depth				*) sampled 43 days after application			
10	L12Aa	20.46 ± 0.27	662.20	31	L22Aa	9.14 ± 0.14	295.89
10	*L12Ab	0.90 ± 0.05	24.90	31	*L22Ab	25.84 ± 2.43	840.74
28	L12Ac	3.93 ± 0.90	127.15	41	*L22Ac	13.47 ± 0.59	422.52
26	L12Ad	9.47 ± 0.66	306.46	29	L22Ad	4.83 ± 0.51	156.48
45	*L12Ae	1.88 ± 0.02	60.81	38	*L22Ae	45.10 ± 2.40	1736.69
16	L12Af	4.06 ± 0.12	131.29	18	L22Af	14.80 ± 1.30	479.05
42	*L12Ag	15.25 ± 0.38	476.60	22	L22Ag	27.35 ± 0.32	885.16
mean = 7.99 ± 7.41 median = 4.06				mean = 20.08 ± 13.76 median = 14.80			
Layer B: 2.5 – 5 cm depth							
10	L12Ba	0.408 ± 0.014	16.69	31	L22Ba	0.077 ± 0.010	3.17
10	*L12Bb	0.013 ± 0.001	0.46	31	*L22Bb	1.061 ± 0.044	47.69
28	L12Bc	0.012 ± 0.001	0.48	41	*L22Bc	0.329 ± 0.005	10.72
26	L12Bd	0.930 ± 0.036	38.05	29	L22Bd	0.394 ± 0.027	16.10
45	*L12Be	0.026 ± 0.002	1.17	38	*L22Be	0.140 ± 0.016	4.78
16	L12Bf	0.269 ± 0.022	10.99	18	L22Bf	0.483 ± 0.033	19.74
42	*L12Bg	1.344 ± 0.196	54.58	22	L22Bg	0.740 ± 0.032	30.29
mean = 0.429 ± 0.520 median = 0.269				mean = 0.461 ± 0.344 median = 0.394			
Layer C: 5 – 10 cm depth							
10	L123a	0.050 ± 0.002	4.22	31	L223a	0.015 ± 0.001	1.23
10	*L123b	< 0,016	0.76	31	*L223b	0.079 ± 0.004	6.68
28	L123c	< 0,012	0.51	41	*L223c	0.034 ± 0.002	2.46
26	L123d	0.166 ± 0.043	14.09	29	L223d	0.147 ± 0.024	11.92
45	*L123e	0.062 ± 0.001	2.68	38	*L223e	0.021 ± 0.001	1.63
16	L123f	0.061 ± 0.002	5.14	18	L223f	0.089 ± 0.008	7.16
42	*L123g	0.076 ± 0.003	8.75	22	L223g	0.198 ± 0.014	16.04
mean = 0.061 ± 0.054 median = 0.061				mean = 0.083 ± 0.069 median = 0.079			

Lindane, continued

TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core	TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core
Layer D: 10 – 20 cm depth							
10	L124a	0.025 ± 0.000	3.24	31	L224a	0.060 ± 0.299	6.98
10	*L124b	n.d.	0.00	31	*L224b	0.039 ± 0.069	4.52
mean = 0.013 ± 0.021				mean = 0.049 ± 0.016			
T3: 140 days after application							
Layer A: 0 – 2.5 cm depth							

10	L13Aa	13.28 ± 1.37	303.06	31	L23Aa	27.94 ± 2.38	561.06
10	L13Ab	3.44 ± 1.11	109.21	31	L23Ab	3.97 ± 0.32	117.75
28	L13Ac	6.56 ± 0.88	163.31	41	L23Ac	37.27 ± 3.08	1052.83
26	L13Ad	15.18 ± 1.89	549.30	29	L23Ad	14.31 ± 2.05	432.31
45	L13Ae	10.01 ± 2.26	296.63	38	L23Ae	20.37 ± 4.20	608.12
16	L13Af	6.25 ± 1.35	253.12	18	L23Af	9.52 ± 1.27	290.84
42	L13Ag	4.18 ± 1.02	131.77	22	L23Ag	15.69 ± 1.63	542.86
mean = 8.60 ± 4.31 median = 6.56				mean = 20.96 ± 10.17 median = 20.44			
Layer B: 2.5 – 5 cm depth							
10	L13Ba	0.308 ± 0.025	10.07	31	L23Ba	17.32 ± 2.226	489.66
10	L13Bb	0.313 ± 0.024	11.45	31	L23Bb	19.77 ± 1.428	508.72
28	L13Bc	0.730 ± 0.055	25.52	41	L23Bc	0.791 ± 0.101	30.57
26	L13Bd	0.294 ± 0.019	6.74	29	L23Bd	1.325 ± 0.162	44.05
45	L13Be	0.320 ± 0.023	8.58	38	L23Be	0.443 ± 0.063	15.86
16	L13Bf	0.327 ± 0.032	9.93	18	L23Bf	0.683 ± 0.124	26.48
42	L13Bg	0.260 ± 0.020	8.15	22	L23Bg	0.444 ± 0.085	16.39
mean = 0.365 ± 0.162 median = 0.313				mean = 0.737 ± 0.362 median = 0.683			
Layer C: 5 – 10 cm depth							
10	L13Ca	0.045 ± 0.012	3.76	31	L233a	1.149 ± 0.093	72.63
10	L13Cb	0.019 ± 0.001	1.83	31	L233b	0.229 ± 0.043	22.28
28	L13Cc	0.039 ± 0.006	3.82	41	L233c	0.247 ± 0.006	18.99
26	L13Cd	0.042 ± 0.001	1.86	29	L233d	0.410 ± 0.015	27.46
45	L13Ce	0.028 ± 0.002	2.13	38	L233e	0.238 ± 0.012	21.47
16	L13Cf	0.036 ± 0.001	2.76	18	L233f	0.414 ± 0.012	26.37
42	L13Cg	0.027 ± 0.004	3.05	22	L233g	0.033 ± 0.001	5.16
mean = 0.034 ± 0.010 median = 0.036				mean = 0.389 ± 0.359 median = 0.247			
Layer D: 10 – 20 cm depth							
10	L13Da	<0,015	1.17	31	L234a	0.187 ± 0.023	26.47
10	L13Db	<0,015	1.27	31	L234b	0.207 ± 0.011	22.18
				mean = 0.197 ± 0.014			
T4: 189 days after application							
Layer A: 0 – 2.5 cm depth							
10	L14A	6.43 ± 0.014	213.44	31	L24Aa	33.45 ± 2.428	844.41
10	L14Ab	15.93 ± 0.675	378.74	31	L24Ab	13.46 ± 0.452	270.52
28	L14Ac	6.83 ± 0.452	120.25	41	L24Ac	30.96 ± 2.393	652.89
26	L14Ad	5.42 ± 0.961	121.22	29	L24Ad	8.49 ± 0.948	242.56
45	L14Ae	7.20 ± 0.646	181.61	38	L24Ae	28.62 ± 1.195	940.68
16	L14Af	7.97 ± 0.165	235.64	18	L24Af	11.29 ± 0.306	323.39
42	L14Ag	7.69 ± 0.602	139.58	22	L24Ag	20.44 ± 3.337	584.83
mean = 8.21 ± 3.51 median = 7.20				mean = 20.96 ± 10.17 median = 20.44			

Lindane, continued

TME	Sample name	Conc. mg/kg dry matter	Lindane in µg /soil core	TME	Sample name	Conc. mg/kg dry matter	Lindane in µg/soil core
Layer B: 2.5 – 5 cm depth							
10	L14Ba	0.047 ± 0.006	2.03	31	L24Ba	2.834 ± 0.206	110.69
10	L14Bb	0.895 ± 0.071	34.73	31	L24Bb	1.604 ± 0.112	52.03
28	L14Bc	1.728 ± 0.020	30.90	41	L24Bc	1.419 ± 0.092	50.83
26	L14Bd	0.805 ± 0.083	27.86	29	L24Bd	0.845 ± 0.035	22.41
45	L14Be	0.305 ± 0.013	9.18	38	L24Be	1.123 ± 0.071	29.36
16	L14Bf	0.159 ± 0.010	5.89	18	L24Bf	0.633 ± 0.081	16.89
42	L14Bg	0.963 ± 0.007	25.50	22	L24Bg	0.452 ± 0.019	13.40
mean = 0.700 ± 0.584 median = 0.805				mean = 1.273 ± 0.802 median = 1.123			
Layer C: 5 – 10 cm depth							
10	L14Ca	n.d.	0.00	31	L24Ca	0.242 ± 0.025	0.00

10	L14Cb	0.056 ± 0.001	4.53	31	L24Cb	0.424 ± 0.038	36.49
mean = 0.030 ± 0.040				mean = 0.333 ± 0.129			
Layer D: 10 – 20 cm depth							
10	L14Da	n.d.	0.00	31	L24Da	0.027 ± 0.008	0.00
10	L14Db	n.d.	0.00	31	L24Db	0.060 ± 0.002	0.00
				mean = 0.044 ± 0.024			
T5: 365 days after application							
Layer A: 0 – 2.5 cm depth							
10	L15Aa	5.28 ± 0.293	154.62	31	L25Aa	20.61 ± 1.60	564.43
10	L15Ab	3.44 ± 0.454	80.12	31	L25Ab	15.25 ± 0.72	309.71
28	L15Ac	4.57 ± 0.091	97.73	41	L25Ac	12.14 ± 2.28	233.53
26	L15Ad	5.08 ± 0.927	112.38	29	L25Ad	7.75 ± 0.89	191.52
45	L15Ae	5.31 ± 0.579	53.77	38	L25Ae	4.32 ± 0.42	96.96
16	L15Af	4.25 ± 0.278	85.85	18	L25Af	14.90 ± 2.70	328.07
42	L15Ag	5.23 ± 0.660	122.61	22	L25Ag	15.98 ± 2.07	388.98
mean = 4.74 ± 0.70 median = 5.09				mean = 12.99 ± 5.46 median = 4.90			
Layer B: 2.5 – 5 cm depth							
10	L15Ba	0.551 ± 0.098	24.56	31	L25Ba	2.911 ± 0.211	131.22
10	L15Bb	0.530 ± 0.045	16.51	31	L25Bb	3.617 ± 0.565	121.50
28	L15Bc	0.470 ± 0.032	11.63	41	L25Bc	1.457 ± 0.138	36.04
26	L15Bd	1.354 ± 0.181	31.96	29	L25Bd	0.905 ± 0.113	30.44
45	L15Be	0.230 ± 0.027	6.05	38	L25Be	2.708 ± 0.220	89.15
16	L15Bf	1.502 ± 0.068	37.83	18	L25Bf	5.109 ± 0.594	103.89
42	L15Bg	0.538 ± 0.046	16.70	22	L25Bg	5.603 ± 0.595	161.72
mean = 0.739 ± 0.485 median = 0.538				mean = 3.187 ± 1.743 median = 2.911			
Layer C: 5 – 10 cm depth							
10	L15Ca	0.020 ± 0.001	2.04	31	L253a	0.383 ± 0.049	30.34
10	L15Cb	0.041 ± 0.012	3.88	31	L253b	0.319 ± 0.037	26.10
28	L15Cc	0.031 ± 0.013	2.61	41	L253c	0.178 ± 0.016	14.86
26	L15Cd	0.036 ± 0.002	2.19	29	L253d	0.474 ± 0.057	36.44
45	L15Ce	0.022 ± 0.003	1.66	38	L253e	0.342 ± 0.019	29.71
16	L15Cf	0.083 ± 0.012	6.08	18	L253f	0.232 ± 0.019	19.98
42	L15Cg	0.022 ± 0.009	1.61	22	L253g	0.429 ± 0.031	37.34
mean = 0.036 ± 0.022 median = 0.031				mean = 0.337 ± 0.105 median = 0.342			
Layer D: 10 – 20 cm depth							
10	L15Da	< 0,008	0.45	31	L254a	< 0,008	0.47
10	L15Db	< 0,008	0.38	31	L254b	< 0,008	0.43

Table Appendix 45: Concentration (Conc.) of Imidacloprid (Imida) in soil ± standard derivation. Not detectable = n.d., below the limit of quantification = < LOQ, n.a. = not analysed. The median of two values is equal to the mean, so it is not shown.

Application of 0,75 kg/ha of Imidacloprid				Application of 20 kg/ha of Imidacloprid			
TME	Sample name	Conc. mg/kg dry matter	Imida in µg/soil core	TME	Sample name	Conc. mg/kg dry matter	Imida in µg/soil core
T0: 1 day after application							
Layer A: 0 – 2.5 cm depth							
20	I10Aa	2.527	50.475	23	I20Ac	5.453	179.111
20	I10Aa	2.189	81.702	49	I20Ad	11.724	373.168
43	I10Ac	1.786	63.139	21	I20Ae	9.149	246.745
13	I10Af	2.369	150.209	11	I20Af	6.687	213.937
3	I10Ag	1.534	148.095	50	I20Ag	12.288	331.931
mean = 2.08 ± 0.41 median = 2.19				mean = 9.06 ± 3.01 median = 9.15			
Layer B: 2.5 – 5 cm depth							
43	I10Bc	< 0.023	0.971	23	I20Bc	0.059	2.454
51	I10Bd	0.249	9.352	49	I20Bd	< 0.022	0.905

4	I10Be	0.251	6.868	21	I20Be	1.082	20.127
13	I10Bf	0.232	9.913	11	I20Bf	0.094	3.799
3	I10Bg	0.570	25.517	50	I20Bg	0.135	4.835
mean = 0.27 ± 0.20 median = 0.25				mean = 0.28 ± 0.45 median = 0.094			
Layer C: 5 – 10 cm depth							
43	I10Cc	n.d.	0.00	23	I20Cc	n.d.	0.00
51	I10Cd	n.d.	0.00	49	I20Cd	n.d.	0.00
T1: 14 days after application							
Layer A: 0 – 2.5 cm depth							
43	I11Ac	4.298	122.469	23	I21Ac	6.716	163.579
51	I11Ad	3.015	68.992	49	I21Ad	2.203	64.772
4	I11Ae	3.092	83.130	21	I21Ae	8.383	247.939
13	I11Af	2.664	67.299	11	I21Af	4.373	114.361
3	I11Ag	4.500	190.372	50	I21Ag	6.982	199.793
mean = 3.15 ± 0.83 median = 17.25				mean = 5.73 ± 2.44 median = 6.72			
Layer B: 2.5 – 5 cm depth							
43	I11Bc	0.182	7.960	23	I21Bc	0.083	2.555
51	I11Bd	< 0.022	0.750	49	I21Bd	0.844	18.508
4	I11Be	0.361	13.504	21	I21Be	0.688	16.332
13	I11Bdf	< 0.021	0.600	11	I21Bf	0.072	2.241
3	I11Bg	< 0.021	0.860	50	I21Bg	0.929	17.508
mean = 0.12 ± 0.15 median = < 0.022				mean = 0.52 ± 0.42 median = 0.688			
Layer C: 5 – 10 cm depth							
43	I11Cc	0.037	3.08	23	I21Cc	0.029	2.93
51	I11Cd	< 0.026	1.24	49	I21Cd	0.064	5.22
mean = 0.03 ± 0.02				mean = 0.05 ± 0.02			
Layer D: 10 – 20 cm depth							
20	I11Da	n.d.	0.00	30	I21Da	<0.026	2.80
20	I11Db	n.d.	0.00	30	I21Db	< 0.026	1.96

Imidacloprid, continued

TME	Sample name	Conc. mg/kg dry matter	Imida in µg/soil core	TME	Sample name	Conc. mg/kg dry matter	Imida in µg/soil core
T2: 42 days after application							
Layer A: 0 – 2.5 cm depth							
43	I12Ac	2.170	65.763	23	I22Ac	5.353	118.377
51	I12Ad	1.586	47.277	49	I22Ad	4.471	119.207
4	I12Ae	1.031	35.892	21	I22Ae	1.830	52.768
13	I12Af	1.881	48.175	11	I22Af	5.077	159.498
3	I12Ag	2.323	77.789	50	I22Ag	4.166	141.288
mean = 1.80 ± 0.51 median = 1.88				mean = 4.18 ± 1.40 median = 4.17			
Layer B: 2.5 – 5 cm depth							
43	I12Bc	0.190	9.673	23	I22Bc	1.534	43.393
51	I12Bd	0.368	12.124	49	I22Bd	1.498	59.200
4	I12Be	0.242	7.594	21	I22Be	< 0.025	0.713
13	I12Bf	< 0.029	0.848	11	I22Bf	1.702	46.204
3	I12Be	0.091	2.427	50	I22Be	0.980	40.070
mean = 0.18 ± 0.13 median = 0.19				mean = 1.15 ± 0.68 median = 1.50			
Layer C: 5 – 10 cm depth							
43	I12Cc	0.028	2.97	23	I12Cc	0.132	12.68
51	I12Cd	0.067	5.99	49	I12Cd	0.107	10.73

mean = 0.05 ± 0.03				mean = 0.12 ± 0.02			
Layer D: 10 – 20 cm depth							
20	I124a	n.d.	0.00	30	I224a	<0.026	2.95
20	I124b	n.d.	0.00	30	I224b	n.d.	0.00
T3: 140 days after application							
Layer A: 0 – 2.5 cm depth							
43	L13Aa	0.393	10.721	23	L23Aa	0.541	21.520
51	L13Ab	0.246	9.145	49	L23Ab	0.748	18.883
4	L13Ac	0.282	8.358	21	L23Ac	0.588	19.486
13	L13Ad	0.362	10.471	11	L23Ad	0.513	17.256
3	L13Ae	0.236	8.996	50	L23Ae	0.530	13.465
mean = 0.30 ± 0.07 median = 0.28				mean = 0.58 ± 0.10 median = 0.54			
Layer B: 2.5 – 5 cm depth							
43	L13Ba	0.456	15.421	23	L23Ba	0.872	18.465
51	L13Bb	0.052	2.205	49	L23Bb	0.032	1.106
4	L13Bc	0.071	2.362	21	L23Bc	0.047	1.112
13	L13Bd	0.443	15.223	11	L23Bd	0.103	4.290
3	L13Be	0.054	1.549	50	L23Be	< 0.024	0.905
mean = 0.22 ± 0.21 median = 0.07				mean = 0.21 ± 0.362 median = 0.47			
Layer C: 5 – 10 cm depth							
43	L13Ca	n.d.	0.00	23	L233a	0.040	3.84
51	L13Cb	n.d.	0.00	49	L233b	0.026	2.58
				mean = 0.03 ± 0.01			
Layer D: 10 – 20 cm depth							
20	L13Da	n.d.	0.00	30	L234a	n.d.	0.00
20	L13Db	n.d.	0.00	30	L234b	n.d.	0.00

TME	Sample name	Conc. mg/kg dry matter	Imida in µg/soil core	TME	Sample name	Conc. mg/kg dry matter	Imida in µg/soil core
T4: 189 days after application							
Layer A: 0 – 2.5 cm depth							
43	L14A	0.612	12.657	23	L24Aa	1.462	34.141
51	L14Ab	0.398	8.181	49	L24Ab	1.230	26.883
4	L14Ac	0.681	11.981	21	L24Ac	1.339	35.277
13	L14Ad	0.436	7.340	11	L24Ad	0.880	16.556
3	L14Ae	0.334	6.028	50	L24Ae	1.023	21.816
mean = 0.49 ± 0.15 median = 0.436				mean = 1.19 ± 0.24 median = 1.23			
Layer B: 2.5 – 5 cm depth							
43	L14Ba	0.052	2.085	23	L24Ba	0.296	8.746
51	L14Bb	0.045	2.091	49	L24Bb	0.241	7.176
4	L14Bc	0.250	9.687	21	L24Bc	0.423	12.847
13	L14Bd	0.168	7.223	11	L24Bd	0.442	13.847
3	L14Bg	< 0.026	1.013	50	L24Bg	0.323	10.292
mean = 0.11 ± 0.10 median = 0.05				mean = 0.35 ± 0.09 median = 0.32			
Layer C: 5 – 10 cm depth							
43	L14Ca	n.d.	0.00	23	L24Ca	0.083	7.56
51	L14Cb	0.060	5.41	49	L24Cb	0.053	5.32
mean = 0.03 ± 0.03				mean = 0.07 ± 0.02			
Layer D: 10 – 20 cm depth							
20	L14Da	n.d.	0.00	30	L24Da	n.d.	0.00

20	L14Db	0.042	5.92		30	L24Db	n.d.	0.00
mean = 0.02 ± 0.02								
T5: 365 days after application								
Layer A: 0 – 2.5 cm depth								
43	L15Aa	0.127	3.018		23	L25Aa	0.684	16.473
51	L15Ab	0.118	2.935		49	L25Ab	0.919	22.446
4	L15Ac	0.113	3.553		21	L25Ac	0.862	18.315
13	L15Ad	0.310	8.376		11	L25Ad	0.670	15.710
3	L15Ae	0.353	8.995		50	L25Ae	0.622	16.094
mean = 0.20 ± 0.12 median = 5.09					mean = 0.75 ± 0.13 median = 0.68			
Layer B: 2.5 – 5 cm depth								
43	I15Ba	0.053	1.699		23	I25Ba	0.532	17.759
51	I15Bb	0.099	2.872		49	I25Bb	0.756	21.117
4	I15Bc	0.064	1.838		21	I25Bc	0.536	13.423
13	I15Bd	0.273	7.348		11	I25Bd	0.384	10.124
3	I15Be	0.216	6.959		50	I25Be	0.220	6.843
mean = 0.14 ± 0.10 median = 0.099					mean = 0.49 ± 0.20 median = 0.53			
Layer C: 5 – 10 cm depth								
43	I15Ca	n.d.	0.00		23	I253a	0.08	6.21
51	I15Cb	n.d.	0.00		49	I253b	0.07	6.83
					mean = 0.08 ± 0.1			
Layer D: 10 – 20 cm depth								
20	I15Da	n.d.	0.00		30	I254a	n.d.	0.00
20	I15Db	n.d.	0.00		30	I254b	< 0.026	2.31

3.9 Watering and leaching in study [2]

Table Appendix 46: Comparison of rainfall/watering and leaching in study [1] (Outdoor) and study [2] (Lab). Given are left: conditions for the TMEs outdoor (TMEs with 1712.9 cm² surface), middle: what is calculated from this values for the Lab-TMEs (78.5 cm² surface), and right: amount of water that was watered or collected from leachate.

May						
Date	Rainfall and watering			Leachate		
	Outdoor mm/m ²	Target Lab ml/TME	Lab ml/TME	Outdoor ml/TME	Target Lab ml/TME	Lab ml/TME
1						
2						
3						
4						
5						
6						
7						
8						
9						
10	5	39				
11	5	39				
12	0	0				
13	0	0				
14	0	0				
15	6	47	40	-	-	-
16	0	0	20	-	-	-
17	0	0		-	-	-
18	0	0	40	-	-	-

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

19	0	0		-	-	-
20	10	79		-	-	-
21	0	0		-	-	-
22	2	16	30	-	-	-
23	3	24		-	-	-
24	0	0	30	-	-	-
25	0	0		-	-	-
26	0	0		-	-	-
27	0	0		-	-	-
28	0	0		-	-	-
29	0	0	40	-	-	-
30	18	141	30	11	0.5	-
31	22	173	40	-	-	-
Sum	61	478.9	270	11	0.5	0

Table Appendix 47: Further details see legend of Table Appendix 46.

June						
	Rainfall and watering			Leachate		
Date	Outdoor mm/m ²	Target Lab ml/TME	Lab ml	Outdoor TME	Target Lab ml/TME	Lab ml/TME
1	0	0	150	-	-	-
2	0	0		-	-	-
3	12	94		-	-	-
4	0	0	120	-	-	-
5	0	0		-	-	-
6	10	79	80	255	11.7	-
7	1	8		-	-	-
8	12	90		11	0.5	-
9	0	0		-	-	-
10	0	0		-	-	-
11	0	0		-	-	-
12	0	0	20	-	-	-
13	0	0		-	-	-
14	8	63		-	-	-
15	0	0	70	-	-	90
16	0	0		-	-	-
17	0	0		-	-	-
18	0	0	20	-	-	-
19	0	0		-	-	-
20	0	0	20	-	-	-
21	33	259		21	1.0	-
22	0	0		-	-	-
23	6	47		-	-	-
24	0	0		-	-	-
25	0	0		-	-	-
26	0	0		-	-	-
27	0	0		-	-	-
28	0	0		-	-	-
29	8	63		28.5	1.3	-
30	0	0		-	-	-
Sum	90	703	480	315.5	14.5	90

Table Appendix 48: Further details see legend of Table Appendix 46.

July						
	Rainfall and watering			Leachate		
Date	Outdoor mm/m ²	Target Lab ml/TME	Lab ml	Outdoor TME	Target Lab ml/TME	Lab ml/TME
1	0	0		-	-	-
2	4.5	35	35	-	-	-
3	0	0		-	-	-
4	1	8	10	-	-	-
5	0	0		-	-	-
6	0	0	15	-	-	-
7	0	0		-	-	-
8	0	0		-	-	-
9	0	0	15	-	-	-
10	0	0		-	-	-
11	0	0		-	-	-
12	0	0	10	-	-	-
13	3.5	27	20	-	-	-
14	6.5	51	20	9	0.4	drops
15	0	0		-	-	-
16	0	0		-	-	-
17	0	0		-	-	-
18	0	0	30	-	-	-
19	16	126	120	-	-	-
20	4.5	35	60	138	6.3	-
21	2	16		-	-	6.7
22	13	102		-	-	-
23	0	0	100	-	-	-
24	9	71	60	-	-	-
25	11	86	60	-	-	-
26	0	0		-	-	1.3
27	0	0	25	-	-	-
28	7	55		37.5	1.7	-
29	0	0		-	-	-
30	0	0	25	-	-	-
31	0	0		-	-	-
Sum	78	612.3	605	185	8.5	8.0

Table Appendix 49: Further details see legend of Table Appendix 46.

August						
	Rainfall and watering			Leachate		
Date	Outdoor mm/m ²	Target Lab ml/TME	Lab ml	Outdoor TME	Target Lab ml/TME	Lab ml/TME
1	0	0		-	-	-
2	0	0		-	-	-
3	3	20	30	-	-	-
4	0	0		-	-	-
5	0	0		-	-	-
6	0	0	30	-	-	-
7	0	0		-	-	-
8	0	0	60	-	-	-
9	39	306	120	50	2.3	-
10	0	0	60	-	-	1.5
11	0	0		-	-	-
12	0	0		-	-	-
13	0	0		-	-	-
14	0	0		-	-	-
15	19	149	90	14.5	0.7	-
16	0	0	190	-	-	-
17	0	0	250	-	-	-
18	1	8	100	5.5	0.3	-
19	50	393		3708	169.9	-
20	0	0	140	-	-	-
21	0	0	140	-	-	129
22	2	16		11	0.5	-
23	0	0		-	-	-
24	0	0	30	-	-	-
25	0	0		-	-	-
26	0	0		-	-	-
27	0	0		-	-	-
28	0	0	30	-	-	-
29	0	0		-	-	-
30	20	157		-	-	-
31	0	0	30	-	-	-
Sum	134	1048	1300	3789	173.6	130.5

Table Appendix 50: Further details see legend of Table Appendix 46.

September						
	Rainfall and watering			Leachate		
Date	Outdoor mm/m ²	Target Lab ml/TME	Lab ml	Outdoor TME	Target Lab ml/TME	Lab ml/TME
1	0	0		-	-	-
2	0	0		-	-	-
3	0	0	40	-	-	-
4	0	0		-	-	-
5	0	0		-	-	-
6	4	31		-	-	-
7	0	0	40	-	-	-
8	0	0		-	-	-
9	0	0		-	-	-
10	0	0	40	-	-	-
11	0	0		-	-	-
12	25	196	40	16.5	0.8	-
13	0	0	40	-	-	-
14	0	0		-	-	-
15	0	0		-	-	-
16	0	0		-	-	-
17	0	0	40	-	-	-
18	0	0		-	-	-
19	0	0	40	-	-	-
20	0	0		-	-	-
21	0	0	40	-	-	-
22	13	102		6	0.3	-
23	0	0		-	-	-
24	0	0	40	-	-	-
25	0	0		-	-	-
26	0	0		-	-	-
27	0	0		-	-	-
28	0	0	40	-	-	-
29	17	133		-	-	-
30	0	0		-	-	-
Sum	59	463.15	400	22.5	1.0311	0

Table Appendix 51: Further details see legend of Table Appendix 46.

October						
	Rainfall and watering			Leachate		
Date	Outdoor mm/m ²	Target Lab ml/TME	Lab ml	Outdoor TME	Target Lab ml/TME	Lab ml/TME
1	0	0		-	-	
2	0	0		-	-	
3	0	0	40	-	-	
4	0	0		-	-	
5	0	0		-	-	
6	0	0		-	-	
7	19	145		179	8.2	
8	0	0	80	-	-	
9	0	0		-	-	7.3
10	0	0	30	-	-	
11	0	0	50	-	-	
12	22	173	50	893	40.9	
13	0	0		-	-	
14	0	0		-	-	
15	0	0	20	-	-	52
16	0	0		-	-	
17	7	51	50	-	-	
18	0	0		-	-	
19	0	0	20	-	-	
20	0	0		-	-	
21	0	0		-	-	
22	0	0		-	-	
23	0	0	30	-	-	
24	0	0		-	-	
25	0	0	40	-	-	
26	5	39	40	559	25.6	
27	0	0		-	-	18
28	0	0		-	-	
29	0	0		-	-	
30	0	0	20	-	-	
31	0	0		-	-	
Sum	52	408.2	470	1631	74.76	77.3

Table Appendix 52: Further details see legend of Table Appendix 46. The high amount which was watered indoor in the beginning of November is due to an failure of the air-conditioning. The temperature between 2nd and 7th of November was about 30 °C.

November						
Datum	Rainfall and watering			Leachate		
	Outdoor mm/m ²	Target Indoor ml/TME	Indoor ml/TME	Outdoor ml/TME	Target Indoor ml/TME	Indoor ml/TME
1	0	0		-	-	-
2	0	0	80	-	-	-
3	0	0		-	-	-
4	0	0		-	-	-
5	0	0	125	-	-	-
6	0	0	100	-	-	-
7	0	0	75	-	-	-
8	0	0		-	-	-
9	0	0		-	-	-
10	0	0		-	-	-
11	0	0		-	-	-
12	0	0		16.5	0.8	-
13	0	0		-	-	-
14	0	0		-	-	-
15	0	0		-	-	-
16	0	0		-	-	-
17	0	0		-	-	-
18	0	0		-	-	-
19	0	0		-	-	-
20	0	0		-	-	-
21						
22						
23						
24						
25						
26						
27						
28						
29						
30						
Sum	0	0	380	16.5	0.8	0

3.10 Results of chemical analyses of Carbendazim in study [3]

Table Appendix 53: Carbendazim contents given as [mg/kg] dry soil for the different replicates on sampling date 1 at day 16 of study [3]

	Content of Carbendazim(mg/ kg dry soil)									
	0-1cm		0-2.5 cm		2.5-5 cm		5-10 cm		10 -20 cm	
	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha
Replicates	4.00	14.00	10.00	14.00	0.025	0.051	0.0064	u.d.l.	u.d.l.	u.d.l.
	8.70	19.00	2.50	9.80	0.072	0.56	u.d.l.	0.26	u.d.l.	u.d.l.
	9.60	57.00	3.90	3.40	0.40	0.026	0.0078	0.010	0.26	u.d.l.
	0.67	17.00	3.90	5.90	0.33	0.026	0.59	u.d.l.	u.d.l.	0.0068
	9.50	8.90	150	3.40	0.24	11	0.074	0.011	0.21	u.d.B
mean	6.49	23.18	4.36	7.30	0.21	0.35	<0.17	<0.09	<0.24	<0.01
stdev.	3.57	17.25	2.96	4.09	0.14	0.43	0.24	0.12	0.03	0.00

Table Appendix 54: Carbendazim contents given as [mg/kg] dry soil for the different replicates on sampling date 2 at day 114 of study [3]

	Content of Carbendazim(mg/ kg dry soil)									
	0-1cm		0-2.5 cm		2.5-5 cm		5-10 cm		10 -20 cm	
	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha
Replicates	0.61	2.10	0.33	0.33	0.020	0.0092	0.018	0.0073	0.0062	0.0059
	0.98	9.30	120	140	0.050	0.011	0.01	0.029	u.d.l.	0.01
	0.41	0.33	0.41	0.30	0.01	0.039	0.0079	0.039	u.d.l.	0.018
	0.15	180	0.19	120	0.04	0.028	0.021	0.083	0.0095	0.0087
	0.41	0.90	0.16	120	0.02	0.14	0.0094	0.025	0.015	0.018
mean	0.51	2.89	0.46	0.89	0.03	0.05	0.01	0.04	<0.01	0.01
stdev.	0.28	3.27	0.38	0.47	0.02	0.05	0.01	0.03	0.004	0.005

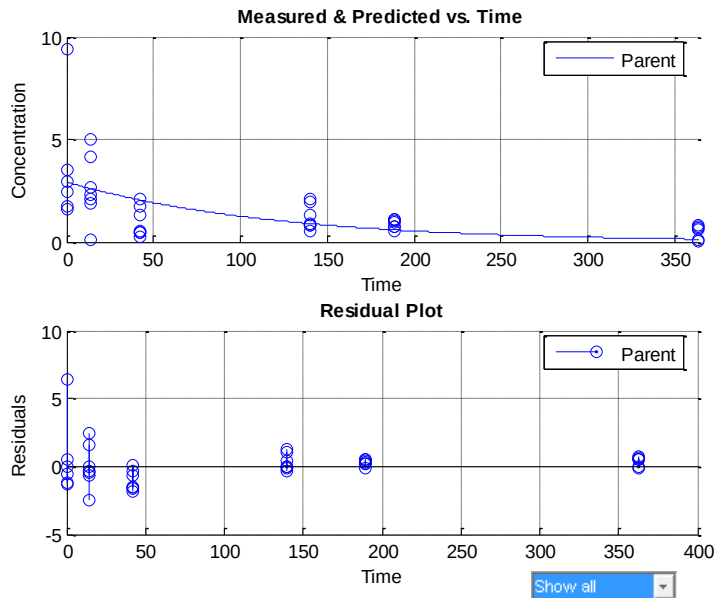
Table Appendix 55: Carbendazim contents given as [mg/kg] dry soil for the different replicates on sampling date 3 at day 148 of study [3]

	Content of Carbendazim(mg/ kg dry soil)									
	0-1cm		0-2.5 cm		2.5-5 cm		5-10 cm		10 -20 cm	
	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha	7,5 kg/ ha	15 kg/ ha
Replicates	u.d.l.	0.08	u.d.l.	0.20	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.
	0.03	0.29	u.d.l.	0.08	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.
	0.01	0.12	0.03	0.09	u.d.l.	0.0083	u.d.l.	u.d.l.	u.d.l.	u.d.l.
	0.04	0.04	u.d.l.	0.14	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.
	0.06	0.01	0.14	0.02	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.	u.d.l.
mean	0.03	0.11	0.09	0.11	-	<0.01	-	-	-	-
stdev.	0.02	0.10	0.06	0.06	-	-	-	-	-	-

4 Appendix: Report files of the exposure simulations

4.1 Disappearance of Lindane in the top 2.5 cm soil assuming SFO kinetics (low rate)

Not normalised



Project: TME Lindan low

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
          Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000         0.0000         Inf
Parent_k:         0.1000         0.0000         Inf
Sink_M(0):         0.0000         0.0000         Inf

# -----
# Chi2 error estimation
# -----
          Parent      Sink
Chi2Err%:    28.2700      NaN
Kinetic Model:    sfo      sink

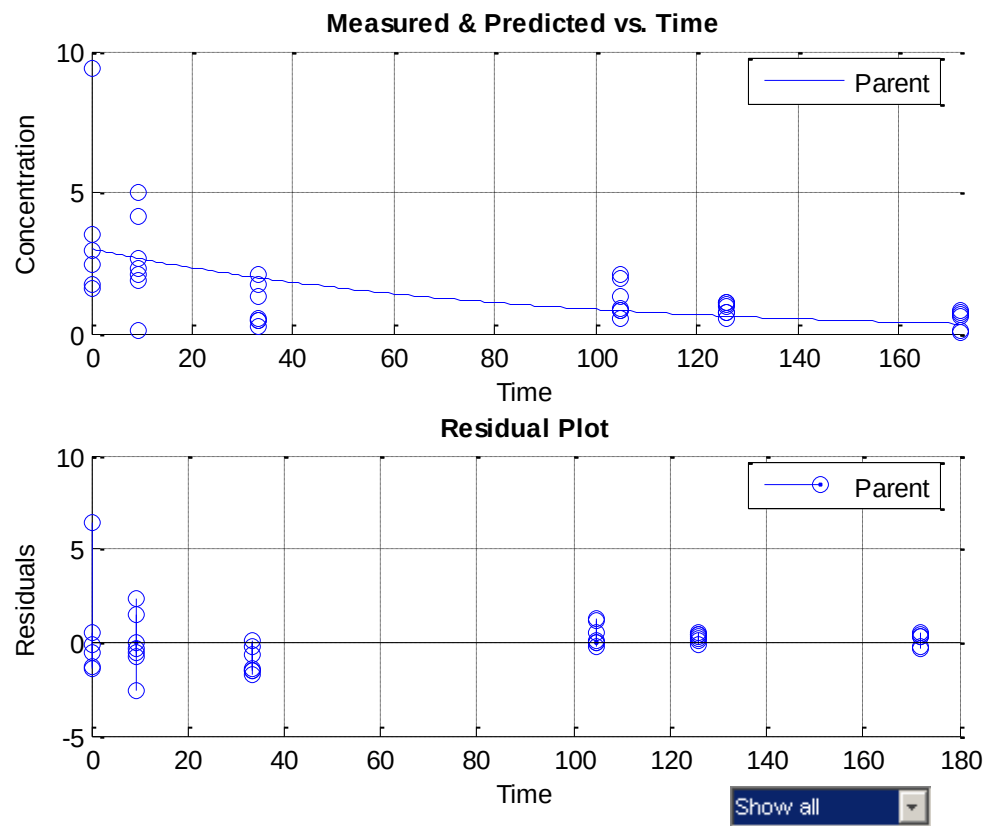
# -----
# Parameter estimation
# -----
Parameter      Estimate      St.Dev      Prob > t
Parent_k        0.0085        0.0032        0.0051
Parent_FFS        1.0000
Parent_M(0)       2.9305        0.4131
Sink_M(0)         0.0000
```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

```
# -----
# DT50 and DT90 values
# -----
          Parent      Sink
      DT50:    81.4475    NaN
      DT90:   270.5628    NaN
Kinetic model:      sfo    sink

# -----
# Measured vs. predicted values
# -----
Time          Compartment Parent          Compartment Sink
      measured predicted residual measured predicted residual
0.0      2.9144      2.9305     -0.0161      NaN      0.0000      NaN
0.0      3.4910      2.9305      0.5605      NaN      0.0000      NaN
0.0      9.3698      2.9305      6.4393      NaN      0.0000      NaN
0.0      1.6188      2.9305     -1.3117      NaN      0.0000      NaN
0.0      2.4300      2.9305     -0.5005      NaN      0.0000      NaN
0.0      1.7103      2.9305     -1.2202      NaN      0.0000      NaN
14.0     5.0175      2.6013      2.4162      NaN      0.3292      NaN
14.0     1.8975      2.6013     -0.7038      NaN      0.3292      NaN
14.0     2.1200      2.6013     -0.4813      NaN      0.3292      NaN
14.0     4.1613      2.6013      1.5600      NaN      0.3292      NaN
14.0     2.2913      2.6013     -0.3100      NaN      0.3292      NaN
14.0     2.6360      2.6013      0.0347      NaN      0.3292      NaN
14.0     0.1141      2.6013     -2.4872      NaN      0.3292      NaN
42.0     0.4928      2.0498     -1.5570      NaN      0.8807      NaN
42.0     1.3425      2.0498     -0.7073      NaN      0.8807      NaN
42.0     0.2533      2.0498     -1.7965      NaN      0.8807      NaN
42.0     0.5561      2.0498     -1.4937      NaN      0.8807      NaN
42.0     2.0943      2.0498      0.0445      NaN      0.8807      NaN
42.0     1.7094      2.0498     -0.3404      NaN      0.8807      NaN
42.0     0.4741      2.0498     -1.5757      NaN      0.8807      NaN
140.0     0.9208      0.8902      0.0306      NaN      2.0402      NaN
140.0     1.9443      0.8902      1.0541      NaN      2.0402      NaN
140.0     1.2980      0.8902      0.4078      NaN      2.0402      NaN
140.0     0.8314      0.8902     -0.0588      NaN      2.0402      NaN
140.0     0.5615      0.8902     -0.3287      NaN      2.0402      NaN
140.0     0.8091      0.8902     -0.0811      NaN      2.0402      NaN
140.0     2.1174      0.8902      1.2272      NaN      2.0402      NaN
189.0     1.0703      0.5867      0.4836      NaN      2.3438      NaN
189.0     0.7779      0.5867      0.1912      NaN      2.3438      NaN
189.0     0.9388      0.5867      0.3521      NaN      2.3438      NaN
189.0     1.0160      0.5867      0.4293      NaN      2.3438      NaN
189.0     1.0815      0.5867      0.4948      NaN      2.3438      NaN
189.0     0.7344      0.5867      0.1477      NaN      2.3438      NaN
189.0     0.5061      0.5867     -0.0806      NaN      2.3438      NaN
363.0     0.6373      0.1334      0.5039      NaN      2.7970      NaN
363.0     0.8139      0.1334      0.6805      NaN      2.7970      NaN
363.0     0.6976      0.1334      0.5642      NaN      2.7970      NaN
363.0     0.7396      0.1334      0.6062      NaN      2.7970      NaN
363.0     0.7268      0.1334      0.5934      NaN      2.7970      NaN
363.0     0.1078      0.1334     -0.0256      NaN      2.7970      NaN
363.0     0.0505      0.1334     -0.0829      NaN      2.7970      NaN
```


Normalised



Project: TME normiert 0-20 cm
Testsystem: Lindane low
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME low.txt

=====
Results of the kinetic evaluation
=====

Initial values

	Initial Value	Lower Bound	Upper Bound
Parent_M(0):	100.0000	0.0000	Inf
Parent_k:	0.1000	0.0000	Inf
Sink_M(0):	0.0000	0.0000	Inf

Chi2 error estimation

	Parent	Sink
Chi2Err%:	25.8566	NaN
Kinetic Model:	sfo	sink

Parameter estimation

Parameter	Estimate	St.Dev	Prob > t
-----------	----------	--------	----------

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

Parent_k	0.0125	0.0041	0.0022
Parent_FFS	1.0000		
Parent_M(0)	2.9932	0.4094	
Sink_M(0)	0.0000		

DT50 and DT90 values

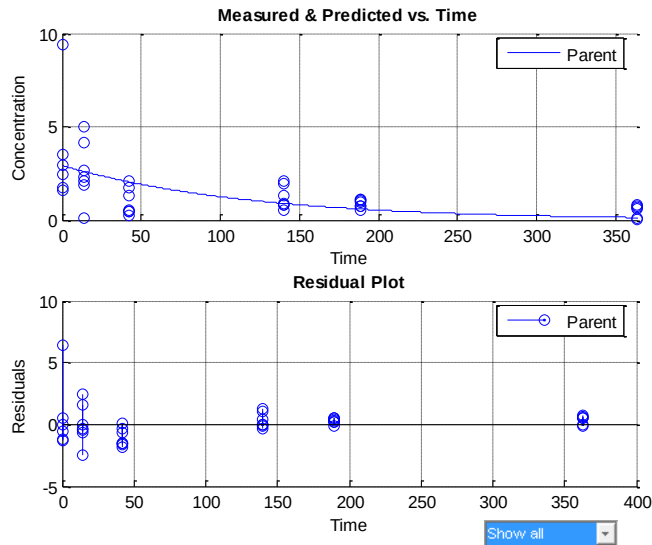
	Parent	Sink
DT50:	55.2654	NaN
DT90:	183.5877	NaN
Kinetic model:	sfo	sink

Measured vs. predicted values

Time	measured	Compartment predicted	Parent residual	measured	Compartment predicted	Sink residual
0.0	2.9144	2.9932	-0.0788	NaN	0.0000	NaN
0.0	3.4910	2.9932	0.4978	NaN	0.0000	NaN
0.0	9.3698	2.9932	6.3766	NaN	0.0000	NaN
0.0	1.6188	2.9932	-1.3744	NaN	0.0000	NaN
0.0	2.4300	2.9932	-0.5632	NaN	0.0000	NaN
0.0	1.7103	2.9932	-1.2829	NaN	0.0000	NaN
9.5	5.0175	2.6577	2.3598	NaN	0.3355	NaN
9.5	1.8975	2.6577	-0.7602	NaN	0.3355	NaN
9.5	2.1200	2.6577	-0.5377	NaN	0.3355	NaN
9.5	4.1613	2.6577	1.5036	NaN	0.3355	NaN
9.5	2.2913	2.6577	-0.3664	NaN	0.3355	NaN
9.5	2.6360	2.6577	-0.0217	NaN	0.3355	NaN
9.5	0.1141	2.6577	-2.5436	NaN	0.3355	NaN
33.2	0.4928	1.9738	-1.4810	NaN	1.0194	NaN
33.2	1.3425	1.9738	-0.6313	NaN	1.0194	NaN
33.2	0.2533	1.9738	-1.7205	NaN	1.0194	NaN
33.2	0.5561	1.9738	-1.4177	NaN	1.0194	NaN
33.2	2.0943	1.9738	0.1205	NaN	1.0194	NaN
33.2	1.7094	1.9738	-0.2644	NaN	1.0194	NaN
33.2	0.4741	1.9738	-1.4997	NaN	1.0194	NaN
104.8	0.9208	0.8045	0.1163	NaN	2.1887	NaN
104.8	1.9443	0.8045	1.1398	NaN	2.1887	NaN
104.8	1.2980	0.8045	0.4935	NaN	2.1887	NaN
104.8	0.8314	0.8045	0.0269	NaN	2.1887	NaN
104.8	0.5615	0.8045	-0.2430	NaN	2.1887	NaN
104.8	0.8091	0.8045	0.0046	NaN	2.1887	NaN
104.8	2.1174	0.8045	1.3129	NaN	2.1887	NaN
126.0	1.0703	0.6161	0.4542	NaN	2.3771	NaN
126.0	0.7779	0.6161	0.1618	NaN	2.3771	NaN
126.0	0.9388	0.6161	0.3227	NaN	2.3771	NaN
126.0	1.0160	0.6161	0.3999	NaN	2.3771	NaN
126.0	1.0815	0.6161	0.4654	NaN	2.3771	NaN
126.0	0.7344	0.6161	0.1183	NaN	2.3771	NaN
126.0	0.5061	0.6161	-0.1100	NaN	2.3771	NaN
172.1	0.6373	0.3458	0.2915	NaN	2.6474	NaN
172.1	0.8139	0.3458	0.4681	NaN	2.6474	NaN
172.1	0.6976	0.3458	0.3518	NaN	2.6474	NaN
172.1	0.7396	0.3458	0.3938	NaN	2.6474	NaN
172.1	0.7268	0.3458	0.3810	NaN	2.6474	NaN
172.1	0.1078	0.3458	-0.2380	NaN	2.6474	NaN
172.1	0.0505	0.3458	-0.2953	NaN	2.6474	NaN

4.2 Disappearance of Lindane in the top 2.5 cm soil assuming HS kinetics (low rate)

Not normalised



Project: TME Lindan low

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000          0.0000          Inf
Parent_k1:         0.1000          0.0000          Inf
Parent_k2:         0.1000          0.0000          Inf
Parent_tb:         0.0000          0.0000          Inf
Sink_M(0):         0.0000          0.0000          Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
Chi2Err%:    35.5753      NaN
Kinetic Model:      hs      sink

# -----
# Parameter estimation
# -----

Parameter      Estimate      St.Dev      Prob > t
Parent_k1       0.8208 >1000.0000      0.5000
Parent_k2       0.0085      0.0036      0.0109
Parent_tb       2.2e-014      NaN      NaN
Parent_FFS       1.0000
Parent_M(0)      2.9300      0.4405
Sink_M(0)        0.0000

# -----
# DT50 and DT90 values
# -----
      Parent      Sink
```

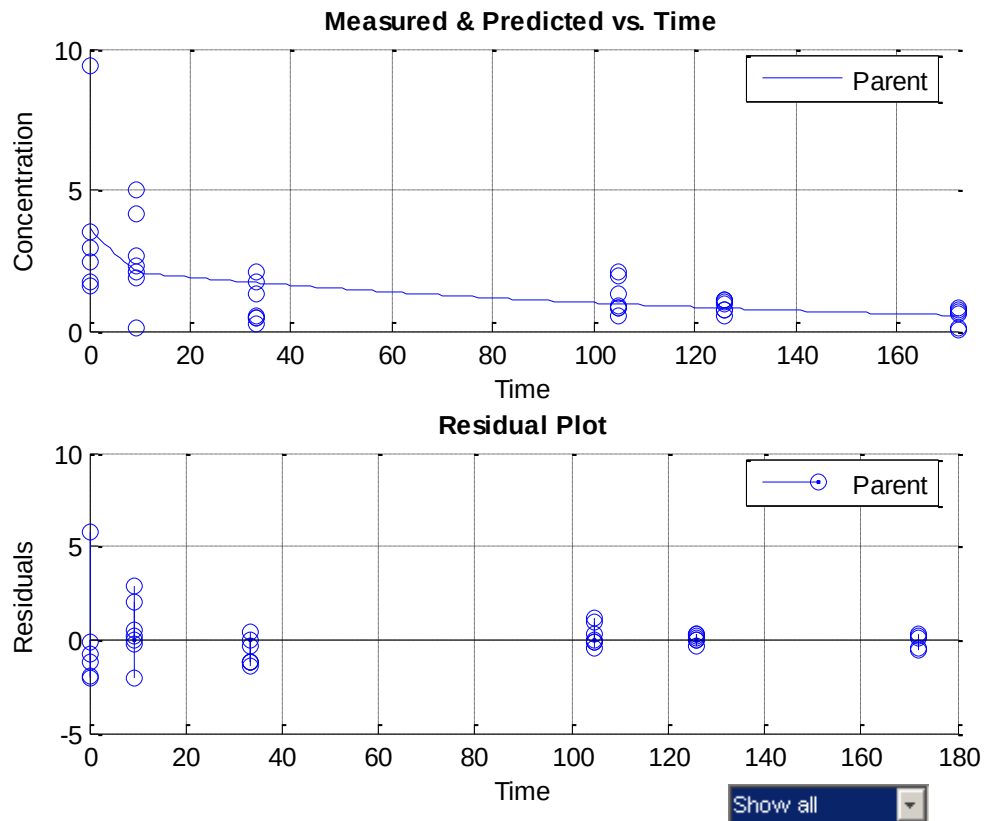
Appendix to the report - Evaluation of the risk for soil organisms under real conditions

DT50: 81.5090 NaN
DT90: 270.7670 NaN
Kinetic model: hs sink

Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	2.9144	2.9300	-0.0156	NaN	0.0000	NaN
0.0	3.4910	2.9300	0.5610	NaN	0.0000	NaN
0.0	9.3698	2.9300	6.4398	NaN	0.0000	NaN
0.0	1.6188	2.9300	-1.3112	NaN	0.0000	NaN
0.0	2.4300	2.9300	-0.5000	NaN	0.0000	NaN
0.0	1.7103	2.9300	-1.2197	NaN	0.0000	NaN
14.0	5.0175	2.6011	2.4164	NaN	0.3289	NaN
14.0	1.8975	2.6011	-0.7036	NaN	0.3289	NaN
14.0	2.1200	2.6011	-0.4811	NaN	0.3289	NaN
14.0	4.1613	2.6011	1.5602	NaN	0.3289	NaN
14.0	2.2913	2.6011	-0.3098	NaN	0.3289	NaN
14.0	2.6360	2.6011	0.0349	NaN	0.3289	NaN
14.0	0.1141	2.6011	-2.4870	NaN	0.3289	NaN
42.0	0.4928	2.0500	-1.5572	NaN	0.8800	NaN
42.0	1.3425	2.0500	-0.7075	NaN	0.8800	NaN
42.0	0.2533	2.0500	-1.7967	NaN	0.8800	NaN
42.0	0.5561	2.0500	-1.4939	NaN	0.8800	NaN
42.0	2.0943	2.0500	0.0443	NaN	0.8800	NaN
42.0	1.7094	2.0500	-0.3406	NaN	0.8800	NaN
42.0	0.4741	2.0500	-1.5759	NaN	0.8800	NaN
140.0	0.9208	0.8909	0.0299	NaN	2.0391	NaN
140.0	1.9443	0.8909	1.0534	NaN	2.0391	NaN
140.0	1.2980	0.8909	0.4071	NaN	2.0391	NaN
140.0	0.8314	0.8909	-0.0595	NaN	2.0391	NaN
140.0	0.5615	0.8909	-0.3294	NaN	2.0391	NaN
140.0	0.8091	0.8909	-0.0818	NaN	2.0391	NaN
140.0	2.1174	0.8909	1.2265	NaN	2.0391	NaN
189.0	1.0703	0.5873	0.4830	NaN	2.3427	NaN
189.0	0.7779	0.5873	0.1906	NaN	2.3427	NaN
189.0	0.9388	0.5873	0.3515	NaN	2.3427	NaN
189.0	1.0160	0.5873	0.4287	NaN	2.3427	NaN
189.0	1.0815	0.5873	0.4942	NaN	2.3427	NaN
189.0	0.7344	0.5873	0.1471	NaN	2.3427	NaN
189.0	0.5061	0.5873	-0.0812	NaN	2.3427	NaN
363.0	0.6373	0.1337	0.5036	NaN	2.7963	NaN
363.0	0.8139	0.1337	0.6802	NaN	2.7963	NaN
363.0	0.6976	0.1337	0.5639	NaN	2.7963	NaN
363.0	0.7396	0.1337	0.6059	NaN	2.7963	NaN
363.0	0.7268	0.1337	0.5931	NaN	2.7963	NaN
363.0	0.1078	0.1337	-0.0259	NaN	2.7963	NaN
363.0	0.0505	0.1337	-0.0832	NaN	2.7963	NaN

Normalised



Project: TME normiert 0-20 cm
Testsystem: Lindane low
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME low.txt

=====
Results of the kinetic evaluation
=====

Initial values

	Initial Value	Lower Bound	Upper Bound
Parent_M(0):	3.6481	0.0000	Inf
Parent_k1:	0.0567	0.0000	Inf
Parent_k2:	0.0081	0.0000	Inf
Parent_tb:	10.0477	0.0000	Inf
Sink_M(0):	0.0000	0.0000	Inf

Chi2 error estimation

	Parent	Sink
Chi2Err%:	23.2890	NaN
Kinetic Model:	hs	sink

Parameter estimation

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

Parameter	Estimate	St.Dev	Prob > t
Parent_k1	0.0567	0.0290	0.0294
Parent_k2	0.0081	0.0037	0.0164
Parent_tb	10.0477	NaN	NaN
Parent_FFS	1.0000		
Parent_M(0)	3.6481	0.5557	
Sink_M(0)	0.0000		

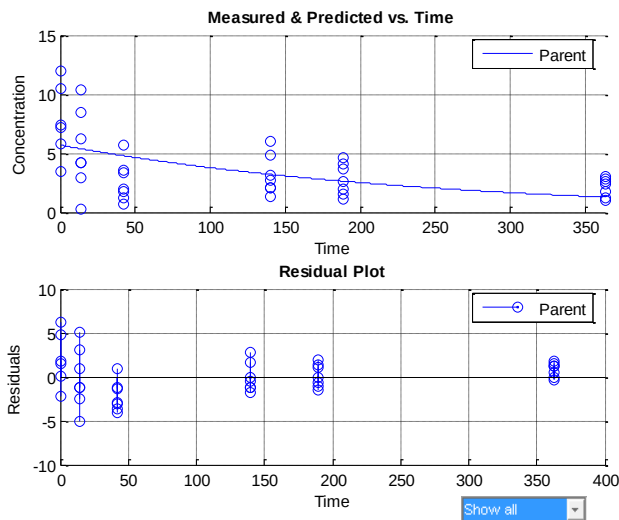
```
# -----
# DT50 and DT90 values
# -----
```

	Parent	Sink
DT50:	25.2814	NaN
DT90:	223.1979	NaN
Kinetic model:	hs	sink

```
# -----
# Measured vs. predicted values
# -----
```

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	2.9144	3.6481	-0.7337	NaN	0.0000	NaN
0.0	3.4910	3.6481	-0.1571	NaN	0.0000	NaN
0.0	9.3698	3.6481	5.7217	NaN	0.0000	NaN
0.0	1.6188	3.6481	-2.0293	NaN	0.0000	NaN
0.0	2.4300	3.6481	-1.2181	NaN	0.0000	NaN
0.0	1.7103	3.6481	-1.9378	NaN	0.0000	NaN
9.5	5.0175	2.1321	2.8854	NaN	1.5160	NaN
9.5	1.8975	2.1321	-0.2346	NaN	1.5160	NaN
9.5	2.1200	2.1321	-0.0121	NaN	1.5160	NaN
9.5	4.1613	2.1321	2.0292	NaN	1.5160	NaN
9.5	2.2913	2.1321	0.1592	NaN	1.5160	NaN
9.5	2.6360	2.1321	0.5039	NaN	1.5160	NaN
9.5	0.1141	2.1321	-2.0180	NaN	1.5160	NaN
33.2	0.4928	1.7103	-1.2175	NaN	1.9378	NaN
33.2	1.3425	1.7103	-0.3678	NaN	1.9378	NaN
33.2	0.2533	1.7103	-1.4570	NaN	1.9378	NaN
33.2	0.5561	1.7103	-1.1542	NaN	1.9378	NaN
33.2	2.0943	1.7103	0.3840	NaN	1.9378	NaN
33.2	1.7094	1.7103	-0.0009	NaN	1.9378	NaN
33.2	0.4741	1.7103	-1.2362	NaN	1.9378	NaN
104.8	0.9208	0.9558	-0.0350	NaN	2.6924	NaN
104.8	1.9443	0.9558	0.9885	NaN	2.6924	NaN
104.8	1.2980	0.9558	0.3422	NaN	2.6924	NaN
104.8	0.8314	0.9558	-0.1244	NaN	2.6924	NaN
104.8	0.5615	0.9558	-0.3943	NaN	2.6924	NaN
104.8	0.8091	0.9558	-0.1467	NaN	2.6924	NaN
104.8	2.1174	0.9558	1.1616	NaN	2.6924	NaN
126.0	1.0703	0.8040	0.2663	NaN	2.8442	NaN
126.0	0.7779	0.8040	-0.0261	NaN	2.8442	NaN
126.0	0.9388	0.8040	0.1348	NaN	2.8442	NaN
126.0	1.0160	0.8040	0.2120	NaN	2.8442	NaN
126.0	1.0815	0.8040	0.2775	NaN	2.8442	NaN
126.0	0.7344	0.8040	-0.0696	NaN	2.8442	NaN
126.0	0.5061	0.8040	-0.2979	NaN	2.8442	NaN
172.1	0.6373	0.5528	0.0845	NaN	3.0953	NaN
172.1	0.8139	0.5528	0.2611	NaN	3.0953	NaN
172.1	0.6976	0.5528	0.1448	NaN	3.0953	NaN
172.1	0.7396	0.5528	0.1868	NaN	3.0953	NaN
172.1	0.7268	0.5528	0.1740	NaN	3.0953	NaN
172.1	0.1078	0.5528	-0.4450	NaN	3.0953	NaN
172.1	0.0505	0.5528	-0.5023	NaN	3.0953	NaN

4.3 Disappearance of Lindane in the top 2.5 cm soil assuming SFO kinetics (high rate)
Not normalised



Project: TME Lindan high

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
          Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000         0.0000         Inf
Parent_k:        0.0000         0.0000         Inf
Sink_M(0):       0.0000         0.0000         Inf

# -----
# Chi2 error estimation
# -----
          Parent      Sink
Chi2Err%:    26.1923    NaN
Kinetic Model:      sfo      sink

# -----
# Parameter estimation
# -----

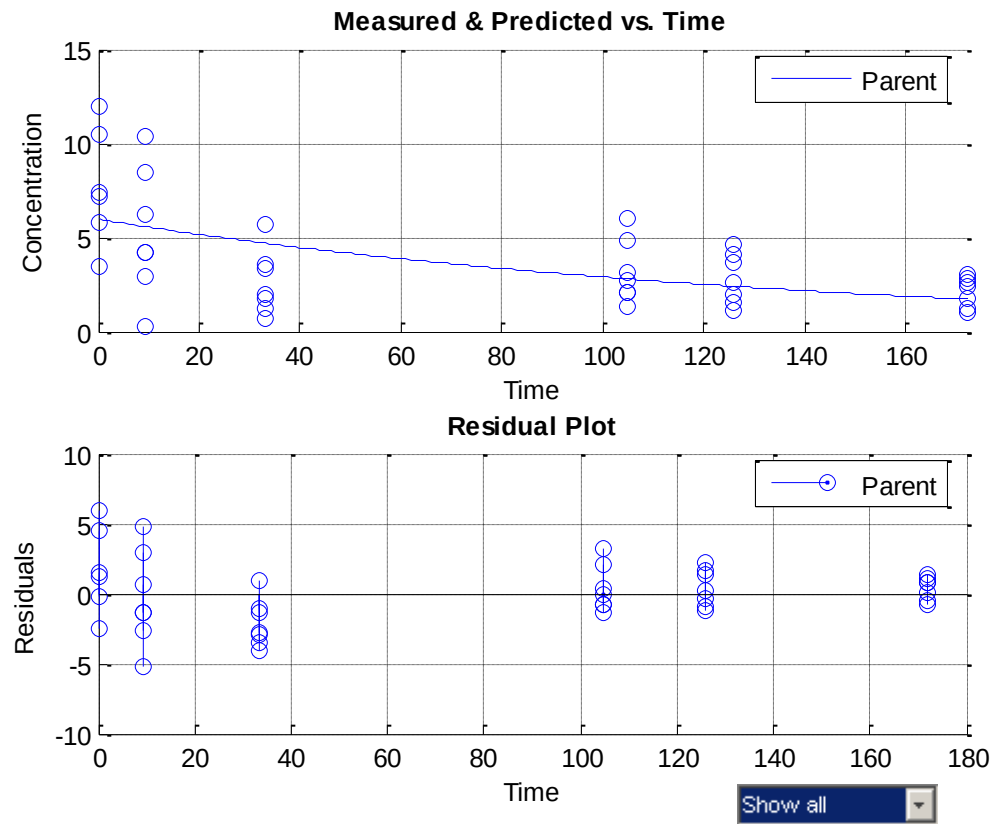
Parameter      Estimate      St.Dev      Prob > t
Parent_k        0.0041        0.0013        0.0017
Parent_FFS       1.0000
Parent_M(0)      5.6906        0.6368
Sink_M(0)        0.0000

# -----
# DT50 and DT90 values
# -----
          Parent      Sink
DT50:        169.5264    NaN
DT90:        563.1545    NaN
Kinetic model:      sfo      sink
```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

# -----						
# Measured vs. predicted values						
# -----						
Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	10.4738	5.6906	4.7832	NaN	0.0000	NaN
0.0	7.4275	5.6906	1.7369	NaN	0.0000	NaN
0.0	7.1525	5.6906	1.4619	NaN	0.0000	NaN
0.0	5.7975	5.6906	0.1069	NaN	0.0000	NaN
0.0	3.4925	5.6906	-2.1981	NaN	0.0000	NaN
0.0	11.9175	5.6906	6.2269	NaN	0.0000	NaN
14.0	8.4434	5.3741	3.0693	NaN	0.3166	NaN
14.0	10.4210	5.3741	5.0469	NaN	0.3166	NaN
14.0	6.2614	5.3741	0.8873	NaN	0.3166	NaN
14.0	4.1730	5.3741	-1.2011	NaN	0.3166	NaN
14.0	2.9303	5.3741	-2.4438	NaN	0.3166	NaN
14.0	4.2065	5.3741	-1.1676	NaN	0.3166	NaN
14.0	0.2970	5.3741	-5.0771	NaN	0.3166	NaN
42.0	1.1859	4.7927	-3.6068	NaN	0.8979	NaN
42.0	3.4030	4.7927	-1.3897	NaN	0.8979	NaN
42.0	1.7334	4.7927	-3.0593	NaN	0.8979	NaN
42.0	0.6898	4.7927	-4.1029	NaN	0.8979	NaN
42.0	5.6603	4.7927	0.8676	NaN	0.8979	NaN
42.0	1.9326	4.7927	-2.8601	NaN	0.8979	NaN
42.0	3.5608	4.7927	-1.2319	NaN	0.8979	NaN
140.0	6.0358	3.2104	2.8254	NaN	2.4802	NaN
140.0	3.1284	3.2104	-0.0820	NaN	2.4802	NaN
140.0	4.8195	3.2104	1.6091	NaN	2.4802	NaN
140.0	2.0566	3.2104	-1.1538	NaN	2.4802	NaN
140.0	2.6611	3.2104	-0.5493	NaN	2.4802	NaN
140.0	1.3795	3.2104	-1.8309	NaN	2.4802	NaN
140.0	2.0256	3.2104	-1.1848	NaN	2.4802	NaN
189.0	4.6093	2.6276	1.9817	NaN	3.0631	NaN
189.0	2.0194	2.6276	-0.6082	NaN	3.0631	NaN
189.0	4.0473	2.6276	1.4197	NaN	3.0631	NaN
189.0	1.1665	2.6276	-1.4611	NaN	3.0631	NaN
189.0	3.7183	2.6276	1.0907	NaN	3.0631	NaN
189.0	1.4904	2.6276	-1.1372	NaN	3.0631	NaN
189.0	2.6114	2.6276	-0.0162	NaN	3.0631	NaN
363.0	3.0354	1.2900	1.7454	NaN	4.4007	NaN
363.0	2.4378	1.2900	1.1478	NaN	4.4007	NaN
363.0	1.7436	1.2900	0.4536	NaN	4.4007	NaN
363.0	1.1999	1.2900	-0.0901	NaN	4.4007	NaN
363.0	0.9638	1.2900	-0.3262	NaN	4.4007	NaN
363.0	2.5591	1.2900	1.2691	NaN	4.4007	NaN
363.0	2.8049	1.2900	1.5149	NaN	4.4007	NaN

Normalised



Project: TME normiert 0-20 cm
Testsystem: Lindane high
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME high.txt

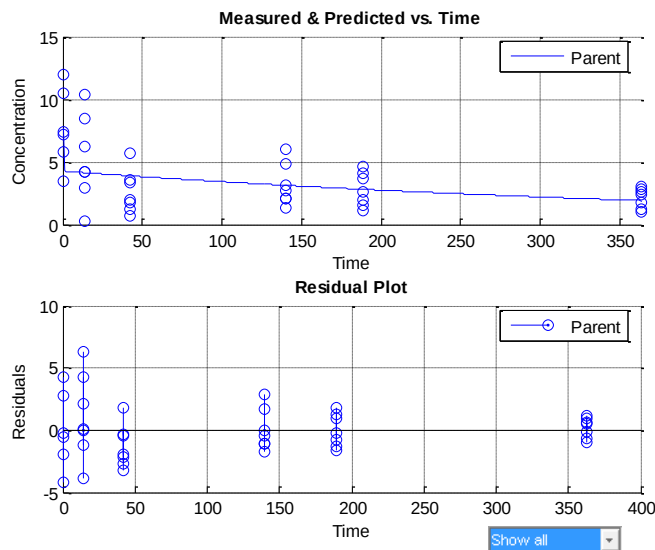
```
# =====  
# Results of the kinetic evaluation  
# =====  
  
# -----  
# Initial values  
# -----  
          Initial Value    Lower Bound    Upper Bound  
Parent_M(0):    5.9581      0.0000      Inf  
Parent_k:       0.0072      0.0000      Inf  
Sink_M(0):      0.0000      0.0000      Inf  
  
# -----  
# Chi2 error estimation  
# -----  
          Parent    Sink  
Chi2Err%:    23.8762    NaN  
Kinetic Model:    sfo    sink  
  
# -----  
# Parameter estimation
```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

```
# -----
#
# Parameter      Estimate      St.Dev      Prob > t
# Parent_k       0.0072       0.0020      4.8e-004
# Parent_FFS     1.0000
# Parent_M(0)    5.9590       0.6505
# Sink_M(0)      0.0000
#
# -----
# DT50 and DT90 values
# -----
#
#           Parent      Sink
# DT50:      96.0869      NaN
# DT90:     319.1937      NaN
# Kinetic model:      sfo      sink
#
# -----
# Measured vs. predicted values
# -----
#
# Time      Compartment Parent      Compartment Sink
# measured predicted residual measured predicted residual
#
# 0.0      10.4738      5.9590      4.5148      NaN      0.0000      NaN
# 0.0       7.4275      5.9590      1.4685      NaN      0.0000      NaN
# 0.0       7.1525      5.9590      1.1935      NaN      0.0000      NaN
# 0.0       5.7975      5.9590     -0.1615      NaN      0.0000      NaN
# 0.0       3.4925      5.9590     -2.4665      NaN      0.0000      NaN
# 0.0      11.9175      5.9590      5.9585      NaN      0.0000      NaN
# 9.5       8.4434      5.5651      2.8783      NaN      0.3939      NaN
# 9.5      10.4210      5.5651      4.8559      NaN      0.3939      NaN
# 9.5       6.2614      5.5651      0.6963      NaN      0.3939      NaN
# 9.5       4.1730      5.5651     -1.3921      NaN      0.3939      NaN
# 9.5       2.9303      5.5651     -2.6348      NaN      0.3939      NaN
# 9.5       4.2065      5.5651     -1.3586      NaN      0.3939      NaN
# 9.5       0.2970      5.5651     -5.2681      NaN      0.3939      NaN
# 33.2      1.1859      4.6899     -3.5040      NaN      1.2691      NaN
# 33.2      3.4030      4.6899     -1.2869      NaN      1.2691      NaN
# 33.2      1.7334      4.6899     -2.9565      NaN      1.2691      NaN
# 33.2      0.6898      4.6899     -4.0001      NaN      1.2691      NaN
# 33.2      5.6603      4.6899      0.9704      NaN      1.2691      NaN
# 33.2      1.9326      4.6899     -2.7573      NaN      1.2691      NaN
# 33.2      3.5608      4.6899     -1.1291      NaN      1.2691      NaN
# 104.8     6.0358      2.7988      3.2370      NaN      3.1602      NaN
# 104.8     3.1284      2.7988      0.3296      NaN      3.1602      NaN
# 104.8     4.8195      2.7988      2.0207      NaN      3.1602      NaN
# 104.8     2.0566      2.7988     -0.7422      NaN      3.1602      NaN
# 104.8     2.6611      2.7988     -0.1377      NaN      3.1602      NaN
# 104.8     1.3795      2.7988     -1.4193      NaN      3.1602      NaN
# 104.8     2.0256      2.7988     -0.7732      NaN      3.1602      NaN
# 126.0     4.6093      2.4007      2.2086      NaN      3.5583      NaN
# 126.0     2.0194      2.4007     -0.3813      NaN      3.5583      NaN
# 126.0     4.0473      2.4007      1.6466      NaN      3.5583      NaN
# 126.0     1.1665      2.4007     -1.2342      NaN      3.5583      NaN
# 126.0     3.7183      2.4007      1.3176      NaN      3.5583      NaN
# 126.0     1.4904      2.4007     -0.9103      NaN      3.5583      NaN
# 126.0     2.6114      2.4007      0.2107      NaN      3.5583      NaN
# 172.1     3.0354      1.7220      1.3134      NaN      4.2370      NaN
# 172.1     2.4378      1.7220      0.7158      NaN      4.2370      NaN
# 172.1     1.7436      1.7220      0.0216      NaN      4.2370      NaN
# 172.1     1.1999      1.7220     -0.5221      NaN      4.2370      NaN
# 172.1     0.9638      1.7220     -0.7582      NaN      4.2370      NaN
# 172.1     2.5591      1.7220      0.8371      NaN      4.2370      NaN
# 172.1     2.8049      1.7220      1.0829      NaN      4.2370      NaN
```

4.4 Disappearance of Lindane in the top 2.5 cm soil assuming HS kinetics (high rate)

Not normalised



```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000          0.0000          Inf
Parent_k1:       0.1000          0.0000          Inf
Parent_k2:       0.1000          0.0000          Inf
Parent_tb:       0.0000          0.0000          Inf
Sink_M(0):       0.0000          0.0000          Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
Chi2Err%:    18.2304      NaN
Kinetic Model:      hs      sink

# -----
# Parameter estimation
# -----
      Parameter      Estimate      St.Dev      Prob > t
Parent_k1      2.2137 >1000.0000      0.5000
Parent_k2      0.0022      0.0012      0.0384
Parent_tb      0.2669 >1000.0000      0.4999
Parent_FFS      1.0000
Parent_M(0)      7.7015      0.9184
Sink_M(0)      0.0000

# -----
# DT50 and DT90 values
# -----
      Parent      Sink
```

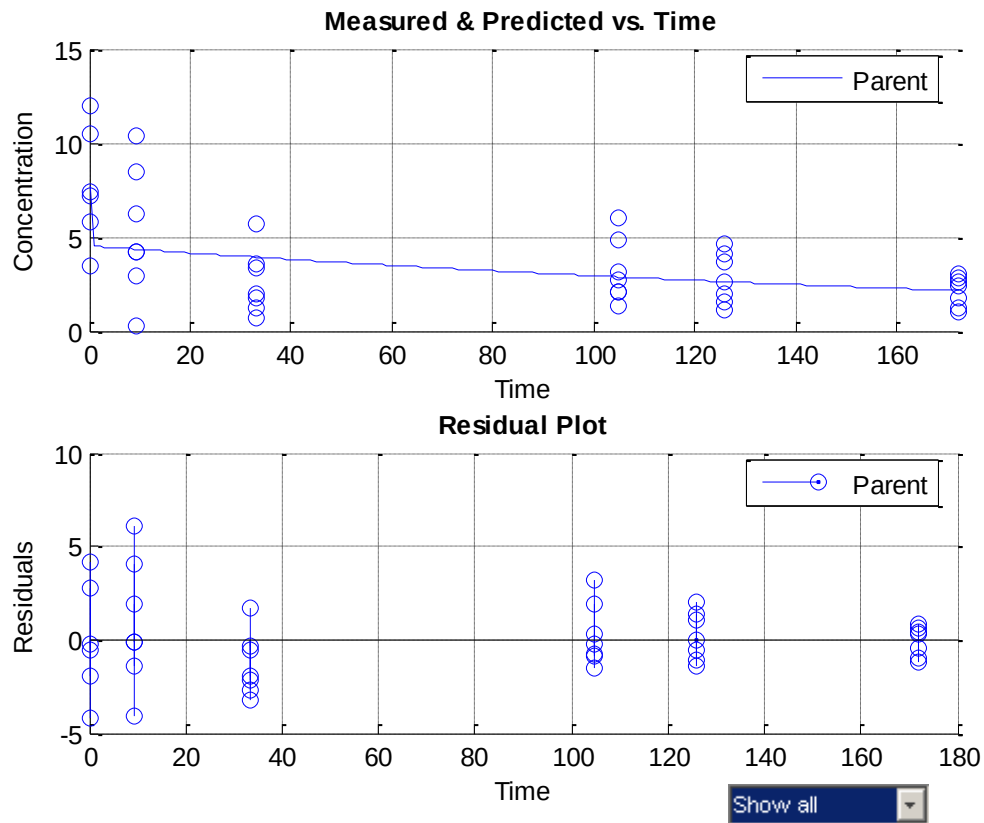
Appendix to the report - Evaluation of the risk for soil organisms under real conditions

DT50: 46.4626 NaN
DT90: 773.7836 NaN
Kinetic model: hs sink

Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	10.4738	7.7015	2.7723	NaN	0.0000	NaN
0.0	7.4275	7.7015	-0.2740	NaN	0.0000	NaN
0.0	7.1525	7.7015	-0.5490	NaN	0.0000	NaN
0.0	5.7975	7.7015	-1.9040	NaN	0.0000	NaN
0.0	3.4925	7.7015	-4.2090	NaN	0.0000	NaN
0.0	11.9175	7.7015	4.2160	NaN	0.0000	NaN
14.0	8.4434	4.1376	4.3058	NaN	3.5640	NaN
14.0	10.4210	4.1376	6.2834	NaN	3.5640	NaN
14.0	6.2614	4.1376	2.1238	NaN	3.5640	NaN
14.0	4.1730	4.1376	0.0354	NaN	3.5640	NaN
14.0	2.9303	4.1376	-1.2073	NaN	3.5640	NaN
14.0	4.2065	4.1376	0.0689	NaN	3.5640	NaN
14.0	0.2970	4.1376	-3.8406	NaN	3.5640	NaN
42.0	1.1859	3.8890	-2.7031	NaN	3.8125	NaN
42.0	3.4030	3.8890	-0.4860	NaN	3.8125	NaN
42.0	1.7334	3.8890	-2.1556	NaN	3.8125	NaN
42.0	0.6898	3.8890	-3.1992	NaN	3.8125	NaN
42.0	5.6603	3.8890	1.7713	NaN	3.8125	NaN
42.0	1.9326	3.8890	-1.9564	NaN	3.8125	NaN
42.0	3.5608	3.8890	-0.3282	NaN	3.8125	NaN
140.0	6.0358	3.1308	2.9050	NaN	4.5707	NaN
140.0	3.1284	3.1308	-0.0024	NaN	4.5707	NaN
140.0	4.8195	3.1308	1.6887	NaN	4.5707	NaN
140.0	2.0566	3.1308	-1.0742	NaN	4.5707	NaN
140.0	2.6611	3.1308	-0.4697	NaN	4.5707	NaN
140.0	1.3795	3.1308	-1.7513	NaN	4.5707	NaN
140.0	2.0256	3.1308	-1.1052	NaN	4.5707	NaN
189.0	4.6093	2.8091	1.8002	NaN	4.8924	NaN
189.0	2.0194	2.8091	-0.7897	NaN	4.8924	NaN
189.0	4.0473	2.8091	1.2382	NaN	4.8924	NaN
189.0	1.1665	2.8091	-1.6426	NaN	4.8924	NaN
189.0	3.7183	2.8091	0.9092	NaN	4.8924	NaN
189.0	1.4904	2.8091	-1.3187	NaN	4.8924	NaN
189.0	2.6114	2.8091	-0.1977	NaN	4.8924	NaN
363.0	3.0354	1.9114	1.1240	NaN	5.7901	NaN
363.0	2.4378	1.9114	0.5264	NaN	5.7901	NaN
363.0	1.7436	1.9114	-0.1678	NaN	5.7901	NaN
363.0	1.1999	1.9114	-0.7115	NaN	5.7901	NaN
363.0	0.9638	1.9114	-0.9476	NaN	5.7901	NaN
363.0	2.5591	1.9114	0.6477	NaN	5.7901	NaN
363.0	2.8049	1.9114	0.8935	NaN	5.7901	NaN

Normalised



Project: TME normiert 0-20 cm
 Testsystem: Lindane high
 Comment:

 KinGUI Version: 1.1

 Input Data: D:\TME\KinGUI\TME high.txt

```

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Initial Value      Lower Bound      Upper Bound
Parent_M(0):      7.7102           0.0000           Inf
Parent_k1:        0.1000           0.0000           Inf
Parent_k2:        0.0033           0.0000           Inf
Parent_tb:       10.0000           0.0000           Inf
Sink_M(0):        0.0000           0.0000           Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
Chi2Err%:  15.4882   NaN
Kinetic Model:      hs      sink

# -----

```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

Parameter estimation

Parameter	Estimate	St.Dev	Prob > t
Parent_k1	0.0593	0.0205	0.0032
Parent_k2	0.0038	0.0021	0.0397
Parent_tb	10.8926	NaN	NaN
Parent_FFS	1.0000		
Parent_M(0)	7.7596	0.9029	
Sink_M(0)	0.0000		

DT50 and DT90 values

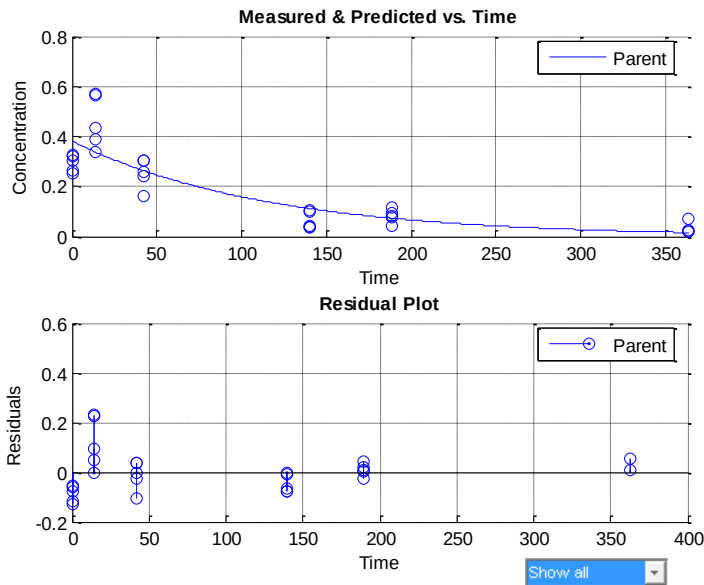
	Parent	Sink
DT50:	23.3514	NaN
DT90:	450.4524	NaN
Kinetic model:	hs	sink

Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	10.4738	7.7596	2.7142	NaN	0.0000	NaN
0.0	7.4275	7.7596	-0.3321	NaN	0.0000	NaN
0.0	7.1525	7.7596	-0.6071	NaN	0.0000	NaN
0.0	5.7975	7.7596	-1.9621	NaN	0.0000	NaN
0.0	3.4925	7.7596	-4.2671	NaN	0.0000	NaN
0.0	11.9175	7.7596	4.1579	NaN	0.0000	NaN
9.5	8.4434	4.4217	4.0217	NaN	3.3378	NaN
9.5	10.4210	4.4217	5.9993	NaN	3.3378	NaN
9.5	6.2614	4.4217	1.8397	NaN	3.3378	NaN
9.5	4.1730	4.4217	-0.2487	NaN	3.3378	NaN
9.5	2.9303	4.4217	-1.4914	NaN	3.3378	NaN
9.5	4.2065	4.4217	-0.2152	NaN	3.3378	NaN
9.5	0.2970	4.4217	-4.1247	NaN	3.3378	NaN
33.2	1.1859	3.7384	-2.5525	NaN	4.0211	NaN
33.2	3.4030	3.7384	-0.3354	NaN	4.0211	NaN
33.2	1.7334	3.7384	-2.0050	NaN	4.0211	NaN
33.2	0.6898	3.7384	-3.0486	NaN	4.0211	NaN
33.2	5.6603	3.7384	1.9219	NaN	4.0211	NaN
33.2	1.9326	3.7384	-1.8058	NaN	4.0211	NaN
33.2	3.5608	3.7384	-0.1776	NaN	4.0211	NaN
104.8	6.0358	2.8548	3.1810	NaN	4.9048	NaN
104.8	3.1284	2.8548	0.2736	NaN	4.9048	NaN
104.8	4.8195	2.8548	1.9647	NaN	4.9048	NaN
104.8	2.0566	2.8548	-0.7982	NaN	4.9048	NaN
104.8	2.6611	2.8548	-0.1937	NaN	4.9048	NaN
104.8	1.3795	2.8548	-1.4753	NaN	4.9048	NaN
104.8	2.0256	2.8548	-0.8292	NaN	4.9048	NaN
126.0	4.6093	2.6349	1.9744	NaN	5.1246	NaN
126.0	2.0194	2.6349	-0.6155	NaN	5.1246	NaN
126.0	4.0473	2.6349	1.4124	NaN	5.1246	NaN
126.0	1.1665	2.6349	-1.4684	NaN	5.1246	NaN
126.0	3.7183	2.6349	1.0834	NaN	5.1246	NaN
126.0	1.4904	2.6349	-1.1445	NaN	5.1246	NaN
126.0	2.6114	2.6349	-0.0235	NaN	5.1246	NaN
172.1	3.0354	2.2151	0.8203	NaN	5.5445	NaN
172.1	2.4378	2.2151	0.2227	NaN	5.5445	NaN
172.1	1.7436	2.2151	-0.4715	NaN	5.5445	NaN
172.1	1.1999	2.2151	-1.0152	NaN	5.5445	NaN
172.1	0.9638	2.2151	-1.2513	NaN	5.5445	NaN
172.1	2.5591	2.2151	0.3440	NaN	5.5445	NaN
172.1	2.8049	2.2151	0.5898	NaN	5.5445	NaN

4.5 Disappearance of imidacloprid e in the top 2.5 cm soil assuming SFO kinetics (low rate)

Not normalised



Project: TME imidcloprid low

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
          Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000         0.0000         Inf
Parent_k:         0.1000         0.0000         Inf
Sink_M(0):         0.0000         0.0000         Inf

# -----
# Chi2 error estimation
# -----
          Parent      Sink
Chi2Err%:    26.0093    NaN
Kinetic Model:    sfo    sink

# -----
# Parameter estimation
# -----

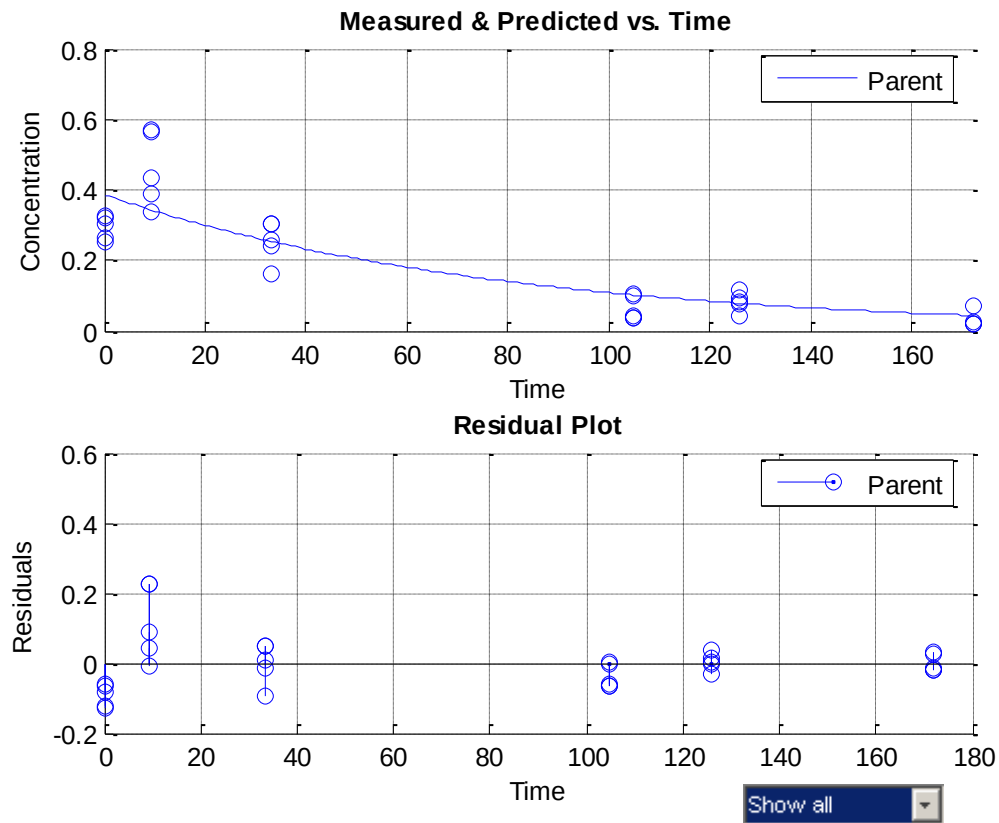
Parameter      Estimate      St.Dev      Prob > t
Parent_k        0.0088        0.0018    1.6e-005
Parent_FFS       1.0000
Parent_M(0)     0.3812        0.0284
Sink_M(0)       0.0000

# -----
# DT50 and DT90 values
# -----
          Parent      Sink
DT50:         79.0546    NaN
DT90:        262.6137    NaN
Kinetic model:    sfo    sink
```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

# -----						
# Measured vs. predicted values						
# -----						
Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.3187	0.3812	-0.0625	NaN	0.0000	NaN
0.0	0.3047	0.3812	-0.0765	NaN	0.0000	NaN
0.0	0.2546	0.3812	-0.1266	NaN	0.0000	NaN
0.0	0.3251	0.3812	-0.0561	NaN	0.0000	NaN
0.0	0.2630	0.3812	-0.1182	NaN	0.0000	NaN
14.0	0.5693	0.3371	0.2322	NaN	0.0440	NaN
14.0	0.3861	0.3371	0.0490	NaN	0.0440	NaN
14.0	0.4316	0.3371	0.0945	NaN	0.0440	NaN
14.0	0.3357	0.3371	-0.0014	NaN	0.0440	NaN
14.0	0.5652	0.3371	0.2281	NaN	0.0440	NaN
42.0	0.3019	0.2637	0.0382	NaN	0.1174	NaN
42.0	0.2609	0.2637	-0.0028	NaN	0.1174	NaN
42.0	0.1590	0.2637	-0.1047	NaN	0.1174	NaN
42.0	0.2387	0.2637	-0.0250	NaN	0.1174	NaN
42.0	0.3017	0.2637	0.0380	NaN	0.1174	NaN
140.0	0.1061	0.1117	-0.0056	NaN	0.2695	NaN
140.0	0.0372	0.1117	-0.0745	NaN	0.2695	NaN
140.0	0.0442	0.1117	-0.0675	NaN	0.2695	NaN
140.0	0.1007	0.1117	-0.0110	NaN	0.2695	NaN
140.0	0.0363	0.1117	-0.0754	NaN	0.2695	NaN
189.0	0.0829	0.0727	0.0102	NaN	0.3085	NaN
189.0	0.0916	0.0727	0.0189	NaN	0.3085	NaN
189.0	0.1163	0.0727	0.0436	NaN	0.3085	NaN
189.0	0.0755	0.0727	0.0028	NaN	0.3085	NaN
189.0	0.0450	0.0727	-0.0277	NaN	0.3085	NaN
363.0	0.0225	0.0158	0.0067	NaN	0.3654	NaN
363.0	0.0271	0.0158	0.0113	NaN	0.3654	NaN
363.0	0.0222	0.0158	0.0064	NaN	0.3654	NaN
363.0	0.0728	0.0158	0.0570	NaN	0.3654	NaN
363.0	0.0712	0.0158	0.0554	NaN	0.3654	NaN

Not normalised



Project: TME normiert 0-20 cm
Testsystem: Imidacloprid low
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME low Imidacloprid.txt

=====
Results of the kinetic evaluation
=====

Initial values

	Initial Value	Lower Bound	Upper Bound
Parent_M(0):	7.7102	0.0000	Inf
Parent_k:	0.0000	0.0000	Inf
Sink_M(0):	0.0000	0.0000	Inf

Chi2 error estimation

	Parent	Sink
Chi2Err%:	24.9202	NaN
Kinetic Model:	sfo	sink

Parameter estimation

Parameter	Estimate	St.Dev	Prob > t
Parent_k	0.0127	0.0023	2.7e-006

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

```

Parent_FFS      1.0000
Parent_M(0)     0.3858      0.0276
Sink_M(0)       0.0000

```

```

# -----
# DT50 and DT90 values
# -----

```

```

          Parent      Sink
DT50:      54.7480      NaN
DT90:     181.8688      NaN
Kinetic model:      sfo      sink

```

```

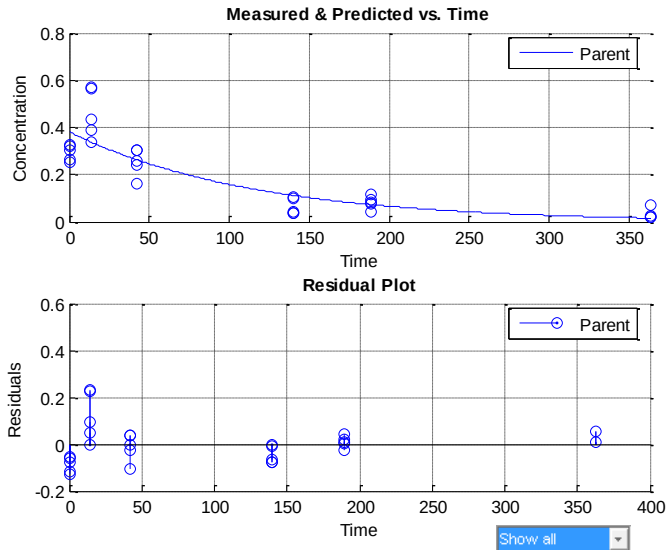
# -----
# Measured vs. predicted values
# -----

```

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.3187	0.3858	-0.0671	NaN	0.0000	NaN
0.0	0.3047	0.3858	-0.0811	NaN	0.0000	NaN
0.0	0.2546	0.3858	-0.1312	NaN	0.0000	NaN
0.0	0.3251	0.3858	-0.0607	NaN	0.0000	NaN
0.0	0.2630	0.3858	-0.1228	NaN	0.0000	NaN
9.5	0.5693	0.3421	0.2272	NaN	0.0436	NaN
9.5	0.3861	0.3421	0.0440	NaN	0.0436	NaN
9.5	0.4316	0.3421	0.0895	NaN	0.0436	NaN
9.5	0.3357	0.3421	-0.0064	NaN	0.0436	NaN
9.5	0.5652	0.3421	0.2231	NaN	0.0436	NaN
33.2	0.3019	0.2534	0.0485	NaN	0.1324	NaN
33.2	0.2609	0.2534	0.0075	NaN	0.1324	NaN
33.2	0.1590	0.2534	-0.0944	NaN	0.1324	NaN
33.2	0.2387	0.2534	-0.0147	NaN	0.1324	NaN
33.2	0.3017	0.2534	0.0483	NaN	0.1324	NaN
104.8	0.1061	0.1024	0.0037	NaN	0.2834	NaN
104.8	0.0372	0.1024	-0.0652	NaN	0.2834	NaN
104.8	0.0442	0.1024	-0.0582	NaN	0.2834	NaN
104.8	0.1007	0.1024	-0.0017	NaN	0.2834	NaN
104.8	0.0363	0.1024	-0.0661	NaN	0.2834	NaN
126.0	0.0829	0.0782	0.0047	NaN	0.3076	NaN
126.0	0.0916	0.0782	0.0134	NaN	0.3076	NaN
126.0	0.1163	0.0782	0.0381	NaN	0.3076	NaN
126.0	0.0755	0.0782	-0.0027	NaN	0.3076	NaN
126.0	0.0450	0.0782	-0.0332	NaN	0.3076	NaN
172.1	0.0225	0.0437	-0.0212	NaN	0.3421	NaN
172.1	0.0271	0.0437	-0.0166	NaN	0.3421	NaN
172.1	0.0222	0.0437	-0.0215	NaN	0.3421	NaN
172.1	0.0728	0.0437	0.0291	NaN	0.3421	NaN
172.1	0.0712	0.0437	0.0275	NaN	0.3421	NaN

4.6 Disappearance of Imidacloprid in the top 2.5 cm soil assuming HS kinetics (low rate)

Not normalised



Project: TME imidcloprid low

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000         0.0000         Inf
Parent_k1:       0.1000         0.0000         Inf
Parent_k2:       0.1000         0.0000         Inf
Parent_tb:       0.0000         0.0000         Inf
Sink_M(0):       0.0000         0.0000         Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
Chi2Err%:    32.7298      NaN
Kinetic Model:      hs      sink

# -----
# Parameter estimation
# -----
      Parameter      Estimate      St.Dev      Prob > t
Parent_k1    5.5e-009 >1000.0000      0.5000
Parent_k2      0.0088      0.0021    1.6e-004
Parent_tb    2.2e-014      NaN      NaN
Parent_FFS      1.0000
Parent_M(0)      0.3812      0.0392
Sink_M(0)      0.0000

# -----
# DT50 and DT90 values
# -----
```

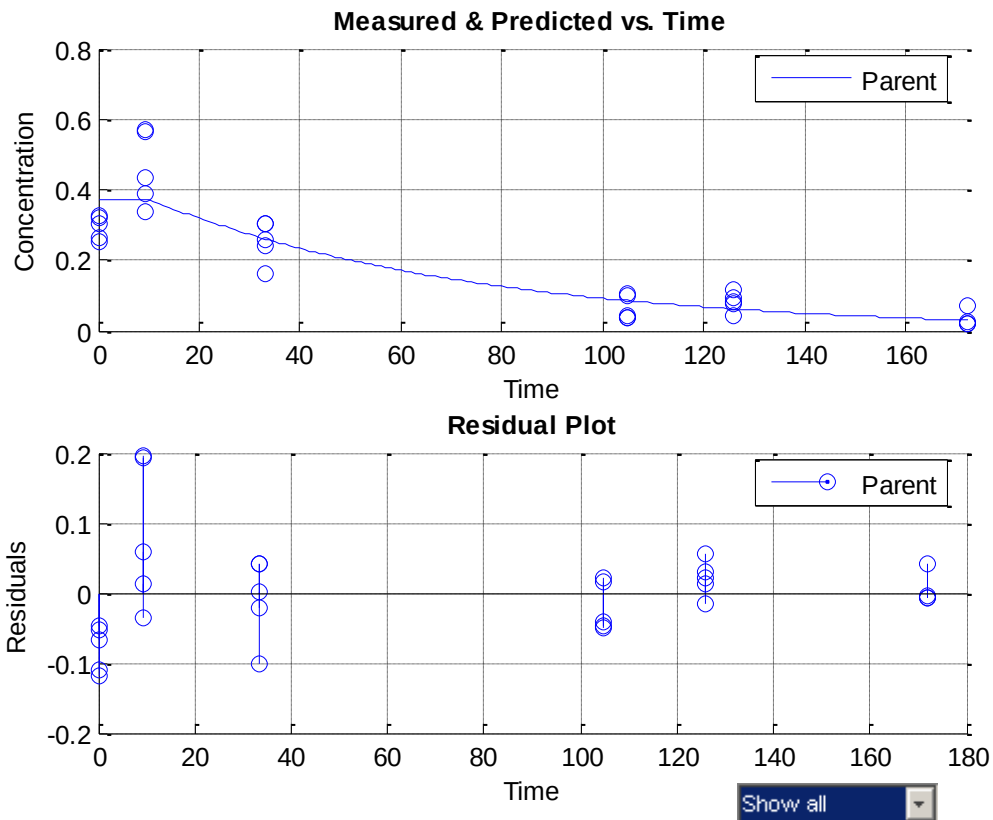
Appendix to the report - Evaluation of the risk for soil organisms under real conditions

	Parent	Sink
DT50:	79.0507	NaN
DT90:	262.6006	NaN
Kinetic model:	hs	sink

Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.3187	0.3812	-0.0625	NaN	0.0000	NaN
0.0	0.3047	0.3812	-0.0765	NaN	0.0000	NaN
0.0	0.2546	0.3812	-0.1266	NaN	0.0000	NaN
0.0	0.3251	0.3812	-0.0561	NaN	0.0000	NaN
0.0	0.2630	0.3812	-0.1182	NaN	0.0000	NaN
14.0	0.5693	0.3372	0.2321	NaN	0.0440	NaN
14.0	0.3861	0.3372	0.0489	NaN	0.0440	NaN
14.0	0.4316	0.3372	0.0944	NaN	0.0440	NaN
14.0	0.3357	0.3372	-0.0015	NaN	0.0440	NaN
14.0	0.5652	0.3372	0.2280	NaN	0.0440	NaN
42.0	0.3019	0.2638	0.0381	NaN	0.1174	NaN
42.0	0.2609	0.2638	-0.0029	NaN	0.1174	NaN
42.0	0.1590	0.2638	-0.1048	NaN	0.1174	NaN
42.0	0.2387	0.2638	-0.0251	NaN	0.1174	NaN
42.0	0.3017	0.2638	0.0379	NaN	0.1174	NaN
140.0	0.1061	0.1117	-0.0056	NaN	0.2695	NaN
140.0	0.0372	0.1117	-0.0745	NaN	0.2695	NaN
140.0	0.0442	0.1117	-0.0675	NaN	0.2695	NaN
140.0	0.1007	0.1117	-0.0110	NaN	0.2695	NaN
140.0	0.0363	0.1117	-0.0754	NaN	0.2695	NaN
189.0	0.0829	0.0727	0.0102	NaN	0.3085	NaN
189.0	0.0916	0.0727	0.0189	NaN	0.3085	NaN
189.0	0.1163	0.0727	0.0436	NaN	0.3085	NaN
189.0	0.0755	0.0727	0.0028	NaN	0.3085	NaN
189.0	0.0450	0.0727	-0.0277	NaN	0.3085	NaN
363.0	0.0225	0.0158	0.0067	NaN	0.3654	NaN
363.0	0.0271	0.0158	0.0113	NaN	0.3654	NaN
363.0	0.0222	0.0158	0.0064	NaN	0.3654	NaN
363.0	0.0728	0.0158	0.0570	NaN	0.3654	NaN
363.0	0.0712	0.0158	0.0554	NaN	0.3654	NaN

Normalised



Project: TME normiert 0-20 cm
Testsystem: Imidacloprid low
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME low Imidacloprid.txt

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Parent_M(0):    7.7102    Lower Bound    Upper Bound
      Parent_k1:     0.0100    0.0000         Inf
      Parent_k2:     0.1000    0.0000         Inf
      Parent_tb:     10.0000    0.0000         Inf
      Sink_M(0):      0.0000    0.0000         Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
      Chi2Err%:   21.7339    NaN
      Kinetic Model:    hs      sink

# -----
# Parameter estimation
# -----
      Parameter    Estimate    St.Dev    Prob > t
```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

Parent_k1	2.7e-014	0.0124	0.5000
Parent_k2	0.0155	0.0028	3.7e-006
Parent_tb	10.0000		
Parent_FFS	1.0000		
Parent_M(0)	0.3728	0.0329	
Sink_M(0)	0.0000		

DT50 and DT90 values

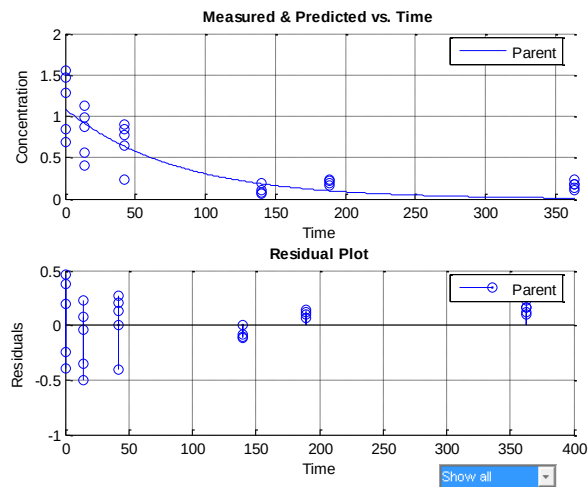
	Parent	Sink
DT50:	54.5859	NaN
DT90:	158.1113	NaN
Kinetic model:	hs	sink

Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.3187	0.3728	-0.0541	NaN	0.0000	NaN
0.0	0.3047	0.3728	-0.0681	NaN	0.0000	NaN
0.0	0.2546	0.3728	-0.1182	NaN	0.0000	NaN
0.0	0.3251	0.3728	-0.0477	NaN	0.0000	NaN
0.0	0.2630	0.3728	-0.1098	NaN	0.0000	NaN
9.5	0.5693	0.3728	0.1965	NaN	0.0000	NaN
9.5	0.3861	0.3728	0.0133	NaN	0.0000	NaN
9.5	0.4316	0.3728	0.0588	NaN	0.0000	NaN
9.5	0.3357	0.3728	-0.0371	NaN	0.0000	NaN
9.5	0.5652	0.3728	0.1924	NaN	0.0000	NaN
33.2	0.3019	0.2599	0.0420	NaN	0.1129	NaN
33.2	0.2609	0.2599	0.0010	NaN	0.1129	NaN
33.2	0.1590	0.2599	-0.1009	NaN	0.1129	NaN
33.2	0.2387	0.2599	-0.0212	NaN	0.1129	NaN
33.2	0.3017	0.2599	0.0418	NaN	0.1129	NaN
104.8	0.1061	0.0854	0.0207	NaN	0.2873	NaN
104.8	0.0372	0.0854	-0.0482	NaN	0.2873	NaN
104.8	0.0442	0.0854	-0.0412	NaN	0.2873	NaN
104.8	0.1007	0.0854	0.0153	NaN	0.2873	NaN
104.8	0.0363	0.0854	-0.0491	NaN	0.2873	NaN
126.0	0.0829	0.0614	0.0215	NaN	0.3114	NaN
126.0	0.0916	0.0614	0.0302	NaN	0.3114	NaN
126.0	0.1163	0.0614	0.0549	NaN	0.3114	NaN
126.0	0.0755	0.0614	0.0141	NaN	0.3114	NaN
126.0	0.0450	0.0614	-0.0164	NaN	0.3114	NaN
172.1	0.0225	0.0300	-0.0075	NaN	0.3428	NaN
172.1	0.0271	0.0300	-0.0029	NaN	0.3428	NaN
172.1	0.0222	0.0300	-0.0078	NaN	0.3428	NaN
172.1	0.0728	0.0300	0.0428	NaN	0.3428	NaN
172.1	0.0712	0.0300	0.0412	NaN	0.3428	NaN

4.7 Disappearance of Imidacloprid in the top 2.5 cm soil assuming SFO kinetics (high rate)

Not normalised



Project: TME imidacloprid high

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
#
# Initial Value      Lower Bound      Upper Bound
Parent_M(0):      100.0000      0.0000      Inf
Parent_k:          0.0000      0.0000      Inf
Sink_M(0):         0.0000      0.0000      Inf

# -----
# Chi2 error estimation
# -----
#
# Parent      Sink
Chi2Err%:     15.6795      NaN
Kinetic Model:      sfo      sink

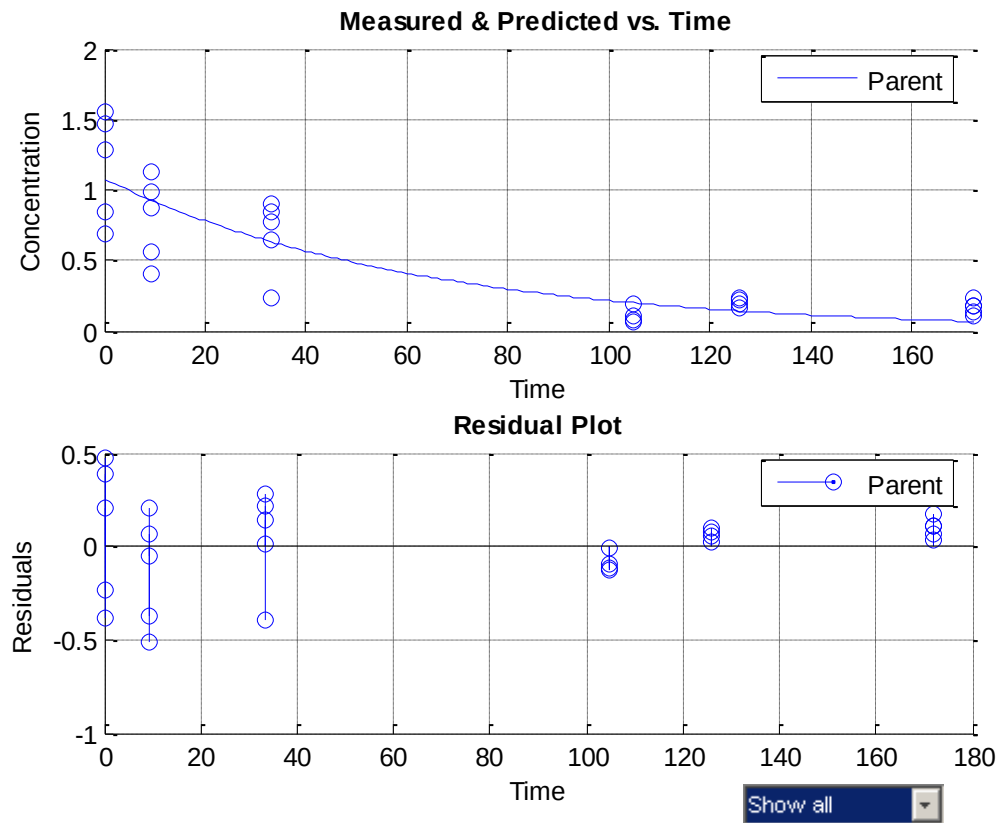
# -----
# Parameter estimation
# -----
#
# Parameter      Estimate      St.Dev      Prob > t
Parent_k         0.0127      0.0028      5.7e-005
Parent_FFS       1.0000
Parent_M(0)      1.0887      0.0858
Sink_M(0)        0.0000

# -----
# DT50 and DT90 values
# -----
#
# Parent      Sink
DT50:         54.5449      NaN
DT90:         181.1943      NaN
Kinetic model:      sfo      sink
```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

# -----						
# Measured vs. predicted values						
# -----						
Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.6890	1.0887	-0.3997	NaN	0.0000	NaN
0.0	1.4682	1.0887	0.3795	NaN	0.0000	NaN
0.0	1.2788	1.0887	0.1901	NaN	0.0000	NaN
0.0	0.8476	1.0887	-0.2411	NaN	0.0000	NaN
0.0	1.5528	1.0887	0.4641	NaN	0.0000	NaN
14.0	0.8702	0.9113	-0.0411	NaN	0.1774	NaN
14.0	0.4098	0.9113	-0.5015	NaN	0.1774	NaN
14.0	1.1338	0.9113	0.2225	NaN	0.1774	NaN
14.0	0.5556	0.9113	-0.3557	NaN	0.1774	NaN
14.0	0.9888	0.9113	0.0775	NaN	0.1774	NaN
42.0	0.9067	0.6384	0.2683	NaN	0.4503	NaN
42.0	0.7729	0.6384	0.1345	NaN	0.4503	NaN
42.0	0.2319	0.6384	-0.4065	NaN	0.4503	NaN
42.0	0.8474	0.6384	0.2090	NaN	0.4503	NaN
42.0	0.6432	0.6384	0.0048	NaN	0.4503	NaN
140.0	0.1865	0.1838	0.0027	NaN	0.9050	NaN
140.0	0.1040	0.1838	-0.0798	NaN	0.9050	NaN
140.0	0.0793	0.1838	-0.1045	NaN	0.9050	NaN
140.0	0.0769	0.1838	-0.1069	NaN	0.9050	NaN
140.0	0.0692	0.1838	-0.1146	NaN	0.9050	NaN
189.0	0.2405	0.0986	0.1419	NaN	0.9901	NaN
189.0	0.1971	0.0986	0.0985	NaN	0.9901	NaN
189.0	0.2203	0.0986	0.1217	NaN	0.9901	NaN
189.0	0.1652	0.0986	0.0666	NaN	0.9901	NaN
189.0	0.1683	0.0986	0.0697	NaN	0.9901	NaN
363.0	0.1729	0.0108	0.1621	NaN	1.0779	NaN
363.0	0.2411	0.0108	0.2303	NaN	1.0779	NaN
363.0	0.1748	0.0108	0.1640	NaN	1.0779	NaN
363.0	0.1318	0.0108	0.1210	NaN	1.0779	NaN
363.0	0.1052	0.0108	0.0944	NaN	1.0779	NaN

Normalised



Project: TME normiert 0-20 cm
Testsystem: Imidacloprid high
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME high Imidacloprid.txt

```

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Initial Value      Lower Bound      Upper Bound
Parent_M(0):      7.7102           0.0000           Inf
Parent_k:          0.0000           0.0000           Inf
Sink_M(0):         0.0000           0.0000           Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
Chi2Err%:  14.0617      NaN
Kinetic Model:    sfo      sink

# -----
# Parameter estimation
# -----
      Parameter      Estimate      St.Dev      Prob > t

```

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

Parent_k	0.0161	0.0032	1.1e-005
Parent_FFS	1.0000		
Parent_M(0)	1.0775	0.0815	
Sink_M(0)	0.0000		

DT50 and DT90 values

	Parent	Sink
DT50:	43.0375	NaN
DT90:	142.9675	NaN
Kinetic model:	sfo	sink

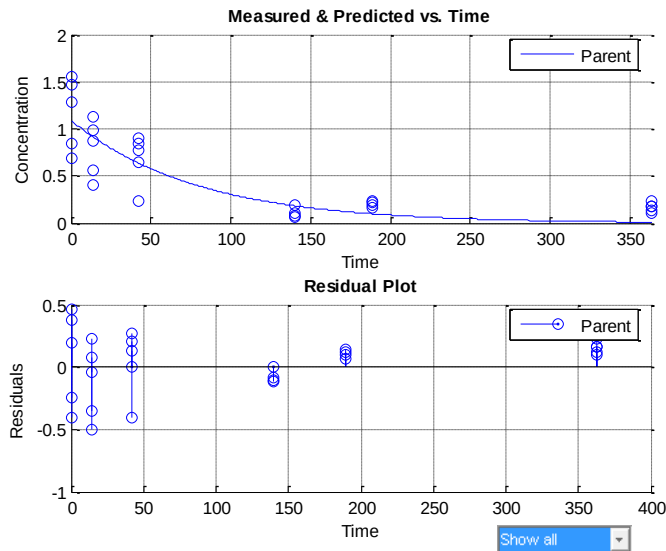
Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.6890	1.0775	-0.3885	NaN	0.0000	NaN
0.0	1.4682	1.0775	0.3907	NaN	0.0000	NaN
0.0	1.2788	1.0775	0.2013	NaN	0.0000	NaN
0.0	0.8476	1.0775	-0.2299	NaN	0.0000	NaN
0.0	1.5528	1.0775	0.4753	NaN	0.0000	NaN
9.5	0.8702	0.9249	-0.0547	NaN	0.1526	NaN
9.5	0.4098	0.9249	-0.5151	NaN	0.1526	NaN
9.5	1.1338	0.9249	0.2089	NaN	0.1526	NaN
9.5	0.5556	0.9249	-0.3693	NaN	0.1526	NaN
9.5	0.9888	0.9249	0.0639	NaN	0.1526	NaN
33.2	0.9067	0.6312	0.2755	NaN	0.4462	NaN
33.2	0.7729	0.6312	0.1417	NaN	0.4462	NaN
33.2	0.2319	0.6312	-0.3993	NaN	0.4462	NaN
33.2	0.8474	0.6312	0.2162	NaN	0.4462	NaN
33.2	0.6432	0.6312	0.0120	NaN	0.4462	NaN
104.8	0.1865	0.1994	-0.0129	NaN	0.8781	NaN
104.8	0.1040	0.1994	-0.0954	NaN	0.8781	NaN
104.8	0.0793	0.1994	-0.1201	NaN	0.8781	NaN
104.8	0.0769	0.1994	-0.1225	NaN	0.8781	NaN
104.8	0.0692	0.1994	-0.1302	NaN	0.8781	NaN
126.0	0.2405	0.1415	0.0990	NaN	0.9359	NaN
126.0	0.1971	0.1415	0.0556	NaN	0.9359	NaN
126.0	0.2203	0.1415	0.0788	NaN	0.9359	NaN
126.0	0.1652	0.1415	0.0237	NaN	0.9359	NaN
126.0	0.1683	0.1415	0.0268	NaN	0.9359	NaN
172.1	0.1729	0.0674	0.1055	NaN	1.0101	NaN
172.1	0.2411	0.0674	0.1737	NaN	1.0101	NaN
172.1	0.1748	0.0674	0.1074	NaN	1.0101	NaN
172.1	0.1318	0.0674	0.0644	NaN	1.0101	NaN
172.1	0.1052	0.0674	0.0378	NaN	1.0101	NaN

4.8 Disappearance of Imidacloprid in the top 2.5 cm soil assuming HS kinetics (high rate)

Not normalised

HS



Project: TME imidacloprid high

KinGUI Version: 1.1

```
# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
      Initial Value      Lower Bound      Upper Bound
Parent_M(0):    100.0000          0.0000          Inf
Parent_k1:       0.1000          0.0000          Inf
Parent_k2:       0.1000          0.0000          Inf
Parent_tb:       0.0000          0.0000          Inf
Sink_M(0):       0.0000          0.0000          Inf

# -----
# Chi2 error estimation
# -----
      Parent      Sink
Chi2Err%:    19.7309      NaN
Kinetic Model:      hs      sink

# -----
# Parameter estimation
# -----
      Parameter      Estimate      St.Dev      Prob > t
Parent_k1          0.1906 >1000.0000      0.5000
Parent_k2          0.0127      0.0035      5.3e-004
Parent_tb          2.2e-014      NaN      NaN
Parent_FFS          1.0000
Parent_M(0)         1.0890      0.1077
Sink_M(0)           0.0000

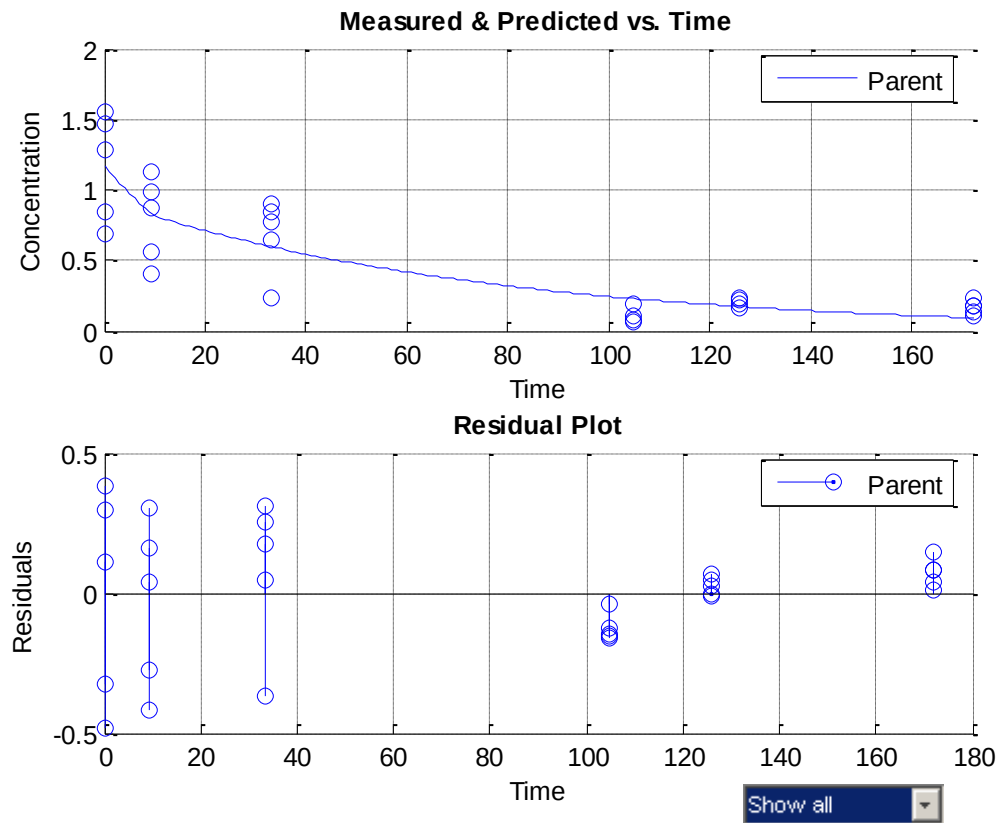
# -----
# DT50 and DT90 values
```

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```
# -----
#                               Parent      Sink
#                               DT50:      54.4645      NaN
#                               DT90:      180.9271     NaN
# Kinetic model:                  hs          sink
```

```
# -----
# Measured vs. predicted values
# -----
# Time          Compartment Parent      Compartment Sink
# measured predicted residual measured predicted residual
0.0      0.6890      1.0890      -0.4000      NaN      0.0000      NaN
0.0      1.4682      1.0890      0.3792      NaN      0.0000      NaN
0.0      1.2788      1.0890      0.1898      NaN      0.0000      NaN
0.0      0.8476      1.0890      -0.2414      NaN      0.0000      NaN
0.0      1.5528      1.0890      0.4638      NaN      0.0000      NaN
14.0     0.8702      0.9113      -0.0411      NaN      0.1777      NaN
14.0     0.4098      0.9113      -0.5015      NaN      0.1777      NaN
14.0     1.1338      0.9113      0.2225      NaN      0.1777      NaN
14.0     0.5556      0.9113      -0.3557      NaN      0.1777      NaN
14.0     0.9888      0.9113      0.0775      NaN      0.1777      NaN
42.0     0.9067      0.6381      0.2686      NaN      0.4509      NaN
42.0     0.7729      0.6381      0.1348      NaN      0.4509      NaN
42.0     0.2319      0.6381      -0.4062      NaN      0.4509      NaN
42.0     0.8474      0.6381      0.2093      NaN      0.4509      NaN
42.0     0.6432      0.6381      0.0051      NaN      0.4509      NaN
140.0    0.1865      0.1833      0.0032      NaN      0.9057      NaN
140.0    0.1040      0.1833      -0.0793      NaN      0.9057      NaN
140.0    0.0793      0.1833      -0.1040      NaN      0.9057      NaN
140.0    0.0769      0.1833      -0.1064      NaN      0.9057      NaN
140.0    0.0692      0.1833      -0.1141      NaN      0.9057      NaN
189.0    0.2405      0.0983      0.1422      NaN      0.9907      NaN
189.0    0.1971      0.0983      0.0988      NaN      0.9907      NaN
189.0    0.2203      0.0983      0.1220      NaN      0.9907      NaN
189.0    0.1652      0.0983      0.0669      NaN      0.9907      NaN
189.0    0.1683      0.0983      0.0700      NaN      0.9907      NaN
363.0    0.1729      0.0107      0.1622      NaN      1.0783      NaN
363.0    0.2411      0.0107      0.2304      NaN      1.0783      NaN
363.0    0.1748      0.0107      0.1641      NaN      1.0783      NaN
363.0    0.1318      0.0107      0.1211      NaN      1.0783      NaN
363.0    0.1052      0.0107      0.0945      NaN      1.0783      NaN
```

Normalised



Project: TME normiert 0-20 cm
Testsystem: Imidacloprid high
Comment:

KinGUI Version: 1.1

Input Data: D:\TME\KinGUI\TME high Imidacloprid.txt

=====
Results of the kinetic evaluation
=====

Initial values

	Initial Value	Lower Bound	Upper Bound
Parent_M(0):	7.7102	0.0000	Inf
Parent_k1:	0.1000	0.0000	Inf
Parent_k2:	0.0100	0.0000	Inf
Parent_tb:	10.0000	0.0000	Inf
Sink_M(0):	0.0000	0.0000	Inf

Chi2 error estimation

	Parent	Sink
Chi2Err%:	12.0026	NaN
Kinetic Model:	hs	sink

Parameter estimation

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Parameter	Estimate	St.Dev	Prob > t
Parent_k1	0.0364	0.0159	0.0152
Parent_k2	0.0134	0.0030	7.0e-005
Parent_tb	10.0000		
Parent_FFS	1.0000		
Parent_M(0)	1.1706	0.0994	
Sink_M(0)	0.0000		

DT50 and DT90 values

	Parent	Sink
DT50:	34.6235	NaN
DT90:	155.0492	NaN
Kinetic model:	hs	sink

Measured vs. predicted values

Time	Compartment Parent			Compartment Sink		
	measured	predicted	residual	measured	predicted	residual
0.0	0.6890	1.1706	-0.4816	NaN	0.0000	NaN
0.0	1.4682	1.1706	0.2976	NaN	0.0000	NaN
0.0	1.2788	1.1706	0.1082	NaN	0.0000	NaN
0.0	0.8476	1.1706	-0.3230	NaN	0.0000	NaN
0.0	1.5528	1.1706	0.3822	NaN	0.0000	NaN
9.5	0.8702	0.8290	0.0412	NaN	0.3417	NaN
9.5	0.4098	0.8290	-0.4192	NaN	0.3417	NaN
9.5	1.1338	0.8290	0.3048	NaN	0.3417	NaN
9.5	0.5556	0.8290	-0.2734	NaN	0.3417	NaN
9.5	0.9888	0.8290	0.1598	NaN	0.3417	NaN
33.2	0.9067	0.5966	0.3101	NaN	0.5741	NaN
33.2	0.7729	0.5966	0.1763	NaN	0.5741	NaN
33.2	0.2319	0.5966	-0.3647	NaN	0.5741	NaN
33.2	0.8474	0.5966	0.2508	NaN	0.5741	NaN
33.2	0.6432	0.5966	0.0466	NaN	0.5741	NaN
104.8	0.1865	0.2292	-0.0427	NaN	0.9414	NaN
104.8	0.1040	0.2292	-0.1252	NaN	0.9414	NaN
104.8	0.0793	0.2292	-0.1499	NaN	0.9414	NaN
104.8	0.0769	0.2292	-0.1523	NaN	0.9414	NaN
104.8	0.0692	0.2292	-0.1600	NaN	0.9414	NaN
126.0	0.2405	0.1725	0.0680	NaN	0.9981	NaN
126.0	0.1971	0.1725	0.0246	NaN	0.9981	NaN
126.0	0.2203	0.1725	0.0478	NaN	0.9981	NaN
126.0	0.1652	0.1725	-0.0073	NaN	0.9981	NaN
126.0	0.1683	0.1725	-0.0042	NaN	0.9981	NaN
172.1	0.1729	0.0932	0.0797	NaN	1.0774	NaN
172.1	0.2411	0.0932	0.1479	NaN	1.0774	NaN
172.1	0.1748	0.0932	0.0816	NaN	1.0774	NaN
172.1	0.1318	0.0932	0.0386	NaN	1.0774	NaN
172.1	0.1052	0.0932	0.0120	NaN	1.0774	NaN

4.9 Inverse modelling: Lindane, low dose, no weighting

PEST RUN RECORD: CASE PEST_SOIL_CONCENTRATIONS

PEST run mode:-

Parameter estimation mode

Case dimensions:-

Number of parameters	:	2
Number of adjustable parameters	:	2
Number of parameter groups	:	2
Number of observations	:	22
Number of prior estimates	:	0

Model command line(s):-

run_pesticide

Jacobian command line:-

na

Model interface files:-

Templates:

PESTICIDE.TPL

for model input files:

LINDANE_7500.PSM

(Parameter values written using single precision protocol.)
(Decimal point always included.)

Instruction files:

PEST.INS

for reading model output files:

PEST_SOIL.PLM

PEST-to-model message file:-

na

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central switch	Multiplier (central)	Method (central)
koc	relative	1.0000E-02	none	switch	2.000	parabolic
kdeg	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound
koc	none	relative	1200.00	100.000	1.000000E+06
kdeg	none	relative	2.670000E-03	2.700000E-04	2.666000E-02

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

Name	Group	Scale	Offset	Model command number
koc	koc	1.00000	0.00000	1
kdeg	kdeg	1.00000	0.00000	1

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	28.4050	1.000	no_name
o2	0.307167	1.000	no_name
o3	0.00000	1.000	no_name
o4	20.6229	1.000	no_name
o5	0.530000	1.000	no_name
o6	0.144286	1.000	no_name
o7	7.99286	1.000	no_name
o8	0.428857	1.000	no_name
o9	6.000000E-02	1.000	no_name
o10	1.500000E-02	1.000	no_name
o11	8.41300	1.000	no_name
o12	0.364571	1.000	no_name
o13	3.371429E-02	1.000	no_name
o14	0.00000	1.000	no_name
o15	8.21043	1.000	no_name
o16	0.700286	1.000	no_name
o17	2.800000E-02	1.000	no_name
o18	0.00000	1.000	no_name
o19	4.73714	1.000	no_name
o20	0.739286	1.000	no_name
o21	3.642857E-02	1.000	no_name
o22	0.00000	1.000	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

OPTIMISATION RECORD

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 340.83

Current parameter values

koc 1200.00

kdeg 2.670000E-03

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 340.83

Lambda = 5.0000 ----->
Phi = 273.25 (0.802 of starting phi)

Lambda = 2.5000 ----->
Phi = 251.00 (0.736 of starting phi)

Lambda = 1.2500 ----->
Phi = 231.99 (0.681 of starting phi)

Lambda = 0.6250 ----->
Phi = 221.49 (0.650 of starting phi)

Lambda = 0.31250 ----->
Phi = 216.50 (0.635 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300

Lowest phi this iteration: 216.50

Current parameter values		Previous parameter values	
koc	3348.00	koc	1200.00
kdeg	2.700000E-04	kdeg	2.670000E-03
Maximum relative change: 1.790		["koc"]	

OPTIMISATION ITERATION NO. : 2
Model calls so far : 8
Starting phi for this iteration: 216.50
parameter "kdeg" frozen: gradient and update vectors out of bounds

Lambda = 0.15625 ----->
Phi = 130.59 (0.603 of starting phi)

Lambda = 7.81250E-02 ----->
Phi = 130.59 (0.603 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300

Lowest phi this iteration: 130.59

Current parameter values		Previous parameter values	
koc	8325.00	koc	3348.00
kdeg	2.700000E-04	kdeg	2.700000E-04
Maximum relative change: 1.487		["koc"]	

OPTIMISATION ITERATION NO. : 3
Model calls so far : 12
Starting phi for this iteration: 130.59
All frozen parameters freed.

Lambda = 7.81250E-02 ----->
Phi = 41.975 (0.321 of starting phi)

Appendix to the report - Evaluation of the risk for soil organisms under real conditions

```
Lambda = 3.90625E-02 ----->
Phi = 41.975 ( 0.321 of starting phi)
```

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 41.975

Current parameter values		Previous parameter values	
koc	18000.0	koc	8325.00
kdeg	1.080000E-03	kdeg	2.700000E-04
Maximum relative change: 3.000		["kdeg"]	

```
OPTIMISATION ITERATION NO.      :    4
Model calls so far              :   16
Starting phi for this iteration:  41.975
```

```
Lambda = 3.90625E-02 ----->
Phi = 23.261 ( 0.554 of starting phi)
```

```
Lambda = 1.95313E-02 ----->
Phi = 23.274 ( 0.554 of starting phi)
```

```
Lambda = 7.81250E-02 ----->
Phi = 23.274 ( 0.554 of starting phi)
```

No more lambdas: phi rising
Lowest phi this iteration: 23.261

Current parameter values		Previous parameter values	
koc	28000.0	koc	18000.0
kdeg	1.120000E-03	kdeg	1.080000E-03
Maximum relative change: 0.5556		["koc"]	

```
OPTIMISATION ITERATION NO.      :    5
Model calls so far              :   21
Starting phi for this iteration:  23.261
```

```
Lambda = 3.90625E-02 ----->
Phi = 23.550 ( 1.012 times starting phi)
```

```
Lambda = 1.95313E-02 ----->
Phi = 23.550 ( 1.012 times starting phi)
```

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 23.550
Relative phi reduction between optimisation iterations less than 0.1000
Switch to central derivatives calculation
(restart from best parameters so far - these achieved at iteration 4)

Current parameter values	
koc	28000.0
kdeg	1.120000E-03

```
OPTIMISATION ITERATION NO.      :    6
Model calls so far              :   25
Starting phi for this iteration:  23.261
```

```
Lambda = 3.90625E-02 ----->
Phi = 23.269 ( 1.000 times starting phi)
```

```
Lambda = 1.95313E-02 ----->
Phi = 23.269 ( 1.000 times starting phi)
```

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No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 23.269

Current parameter values		Previous parameter values	
koc	28000.0	koc	28000.0
kdeg	1.140000E-03	kdeg	1.120000E-03

Maximum relative change: 1.7857E-02 ["kdeg"]

OPTIMISATION ITERATION NO. : 7
Model calls so far : 31
Starting phi for this iteration: 23.269

Lambda = 1.95313E-02 ----->
Phi = 23.256 (0.999 of starting phi)

Lambda = 9.76563E-03 ----->
Phi = 23.256 (0.999 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 23.256

Current parameter values		Previous parameter values	
koc	28000.0	koc	28000.0
kdeg	1.160000E-03	kdeg	1.140000E-03

Maximum relative change: 1.7544E-02 ["kdeg"]

Optimisation complete: the 3 lowest phi's are within a relative distance
of eachother of 1.000E-02
Total model calls: 37

The model has been run one final time using best parameters.
Thus all model input files contain best parameter values, and model
output files contain model results based on these parameters.

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	28000.0	20997.8	35002.2
kdeg	1.160000E-03	-2.672482E-04	2.587248E-03

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in
parameter space as the confidence limits themselves - see PEST manual.

See file PEST_SOIL_CONCENTRATIONS.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	28.4050	27.0320	1.37300	1.000	no_name
o2	0.307167	0.00000	0.307167	1.000	no_name
o3	0.00000	0.00000	0.00000	1.000	no_name
o4	20.6229	18.5000	2.12286	1.000	no_name
o5	0.530000	2.000000E-03	0.528000	1.000	no_name
o6	0.144286	0.00000	0.144286	1.000	no_name
o7	7.99286	10.9920	-2.99914	1.000	no_name
o8	0.428857	1.200000E-02	0.416857	1.000	no_name
o9	6.000000E-02	0.00000	6.000000E-02	1.000	no_name

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o10	1.500000E-02	0.00000	1.500000E-02	1.000	no_name
o11	8.41300	7.06300	1.35000	1.000	no_name
o12	0.364571	3.600000E-02	0.328571	1.000	no_name
o13	3.371429E-02	0.00000	3.371429E-02	1.000	no_name
o14	0.00000	0.00000	0.00000	1.000	no_name
o15	8.21043	6.79800	1.41243	1.000	no_name
o16	0.700286	4.400000E-02	0.656286	1.000	no_name
o17	2.800000E-02	0.00000	2.800000E-02	1.000	no_name
o18	0.00000	0.00000	0.00000	1.000	no_name
o19	4.73714	6.32600	-1.58886	1.000	no_name
o20	0.739286	9.600000E-02	0.643286	1.000	no_name
o21	3.642857E-02	0.00000	3.642857E-02	1.000	no_name
o22	0.00000	0.00000	0.00000	1.000	no_name

See file PEST_SOIL_CONCENTRATIONS.RES for more details of residuals in graph-ready format.

See file PEST_SOIL_CONCENTRATIONS.SEO for composite observation sensitivities.

Objective function ----->

Sum of squared weighted residuals (ie phi) = 23.26

Correlation Coefficient ----->

Correlation coefficient = 0.9909

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	=	22
Mean value of non-zero weighted residuals	=	0.2213
Maximum weighted residual [observation "o4"]	=	2.123
Minimum weighted residual [observation "o7"]	=	-2.999
Standard variance of weighted residuals	=	1.163
Standard error of weighted residuals	=	1.078

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.)
If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	1.1268E+07	0.5900
kdeg	0.5900	4.6813E-07

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	0.2569
kdeg	0.2569	1.000

Normalized eigenvectors of parameter covariance matrix ----->

Vector_1	Vector_2

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koc	5.2362E-08	-1.000
kdeg	-1.000	-5.2362E-08

Eigenvalues ----->

4.3772E-07	1.1268E+07
------------	------------

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	28000.0	20997.8	35002.2
DT50	597.54	267.91	-2593.65

Minimum error for which the Chi²-Test passes according to FOCUS: 23.15 %

4.10 Inverse modelling: Lindane, low dose, data weighting

PEST RUN RECORD: CASE PEST_SOIL_CONCENTRATIONS

PEST run mode:-

Parameter estimation mode

Case dimensions:-

Number of parameters	:	2
Number of adjustable parameters	:	2
Number of parameter groups	:	2
Number of observations	:	22
Number of prior estimates	:	0

Model command line(s):-

run_pesticide

Jacobian command line:-

na

Model interface files:-

Templates:

PESTICIDE.TPL

for model input files:

LINDANE_7500.PSM

(Parameter values written using single precision protocol.)

(Decimal point always included.)

Instruction files:

PEST.INS

for reading model output files:

PEST_SOIL.PLM

PEST-to-model message file:-

na

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central	Multiplier (central)	Method (central)
koc	relative	1.0000E-02	none	switch	2.000	parabolic
kdeg	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound
koc	none	relative	1200.00	100.000	1.000000E+06
kdeg	none	relative	2.670000E-03	2.700000E-04	2.666000E-02

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Name	Group	Scale	Offset	Model command number
koc	koc	1.00000	0.00000	1
kdeg	kdeg	1.00000	0.00000	1

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	28.4050	1.000	no_name
o2	0.307167	30.00	no_name
o3	0.00000	60.00	no_name
o4	20.6229	1.000	no_name
o5	0.530000	30.00	no_name
o6	0.144286	60.00	no_name
o7	7.99286	5.000	no_name
o8	0.428857	30.00	no_name
o9	6.000000E-02	60.00	no_name
o10	1.500000E-02	30.00	no_name
o11	8.41300	5.000	no_name
o12	0.364571	30.00	no_name
o13	3.371429E-02	60.00	no_name
o14	0.00000	30.00	no_name
o15	8.21043	5.000	no_name
o16	0.700286	30.00	no_name
o17	2.800000E-02	60.00	no_name
o18	0.00000	30.00	no_name
o19	4.73714	5.000	no_name
o20	0.739286	30.00	no_name
o21	3.642857E-02	60.00	no_name
o22	0.00000	30.00	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

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OPTIMISATION RECORD

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 2264.5

Current parameter values

koc 1200.00

kdeg 2.670000E-03

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 2264.5

Lambda = 5.0000 ----->
Phi = 1909.4 (0.843 of starting phi)

Lambda = 2.5000 ----->
Phi = 1759.1 (0.777 of starting phi)

Lambda = 1.2500 ----->
Phi = 1555.3 (0.687 of starting phi)

Lambda = 0.62500 ----->
Phi = 1371.1 (0.606 of starting phi)

Lambda = 0.31250 ----->
Phi = 1269.0 (0.560 of starting phi)

Lambda = 0.15625 ----->
Phi = 1227.6 (0.542 of starting phi)

Lambda = 7.81250E-02 ----->
Phi = 1214.3 (0.536 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 1214.3

Current parameter values		Previous parameter values	
koc	2120.00	koc	1200.00
kdeg	1.610000E-03	kdeg	2.670000E-03
Maximum relative change: 0.7667		["koc"]	

OPTIMISATION ITERATION NO. : 2
Model calls so far : 10
Starting phi for this iteration: 1214.3

Lambda = 3.90625E-02 ----->
Phi = 961.15 (0.792 of starting phi)

Lambda = 1.95313E-02 ----->
Phi = 961.15 (0.792 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 961.15

Current parameter values		Previous parameter values	
koc	2957.00	koc	2120.00
kdeg	7.800000E-04	kdeg	1.610000E-03
Maximum relative change: 0.5155		["kdeg"]	

OPTIMISATION ITERATION NO. : 3

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Model calls so far : 14
Starting phi for this iteration: 961.15

Lambda = 1.95313E-02 ----->
Phi = 920.67 (0.958 of starting phi)

Lambda = 9.76563E-03 ----->
Phi = 920.67 (0.958 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 920.67
Relative phi reduction between optimisation iterations less than 0.1000
Switch to central derivatives calculation

Current parameter values		Previous parameter values	
koc	3382.00	koc	2957.00
kdeg	5.000000E-04	kdeg	7.800000E-04
Maximum relative change: 0.3590		["kdeg"]	

OPTIMISATION ITERATION NO. : 4
Model calls so far : 18
Starting phi for this iteration: 920.67

Lambda = 9.76563E-03 ----->
Phi = 910.96 (0.989 of starting phi)

Lambda = 4.88281E-03 ----->
Phi = 910.93 (0.989 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 910.93

Current parameter values		Previous parameter values	
koc	3664.00	koc	3382.00
kdeg	2.700000E-04	kdeg	5.000000E-04
Maximum relative change: 0.4600		["kdeg"]	

OPTIMISATION ITERATION NO. : 5
Model calls so far : 24
Starting phi for this iteration: 910.93

Lambda = 2.44141E-03 ----->
Phi = 910.81 (1.000 of starting phi)

Lambda = 1.22070E-03 ----->
Phi = 910.81 (1.000 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 910.81

Current parameter values		Previous parameter values	
koc	3675.00	koc	3664.00
kdeg	2.800000E-04	kdeg	2.700000E-04
Maximum relative change: 3.7037E-02		["kdeg"]	

OPTIMISATION ITERATION NO. : 6
Model calls so far : 30
Starting phi for this iteration: 910.81

Lambda = 1.22070E-03 ----->
Phi = 910.76 (1.000 of starting phi)

Lambda = 6.10352E-04 ----->

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```

Phi = 910.76      ( 1.000 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 910.76

Current parameter values          Previous parameter values
koc          3676.00              koc          3675.00
kdeg         2.800000E-04         kdeg         2.800000E-04
Maximum relative change: 2.7211E-04 ["koc"]

Optimisation complete: the 3 lowest phi's are within a relative distance
                        of eachother of 1.000E-02
Total model calls: 36

The model has been run one final time using best parameters.
Thus all model input files contain best parameter values, and model
output files contain model results based on these parameters.

```

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	3676.00	2036.92	5315.08
kdeg	2.800000E-04	-1.336517E-03	1.896517E-03

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in
parameter space as the confidence limits themselves - see PEST manual.

See file PEST_SOIL_CONCENTRATIONS.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	28.4050	21.5860	6.81900	1.000	no_name
o2	0.307167	0.00000	0.307167	30.00	no_name
o3	0.00000	0.00000	0.00000	60.00	no_name
o4	20.6229	8.08700	12.5359	1.000	no_name
o5	0.530000	2.900000E-02	0.501000	30.00	no_name
o6	0.144286	0.00000	0.144286	60.00	no_name
o7	7.99286	7.62800	0.364857	5.000	no_name
o8	0.428857	0.129000	0.299857	30.00	no_name
o9	6.000000E-02	0.00000	6.000000E-02	60.00	no_name
o10	1.500000E-02	0.00000	1.500000E-02	30.00	no_name
o11	8.41300	7.05700	1.35600	5.000	no_name
o12	0.364571	0.367000	-2.428571E-03	30.00	no_name
o13	3.371429E-02	2.000000E-03	3.171429E-02	60.00	no_name
o14	0.00000	0.00000	0.00000	30.00	no_name
o15	8.21043	6.87100	1.33943	5.000	no_name
o16	0.700286	0.447000	0.253286	30.00	no_name
o17	2.800000E-02	4.000000E-03	2.400000E-02	60.00	no_name
o18	0.00000	0.00000	0.00000	30.00	no_name
o19	4.73714	6.01500	-1.27786	5.000	no_name
o20	0.739286	0.916000	-0.176714	30.00	no_name
o21	3.642857E-02	2.200000E-02	1.442857E-02	60.00	no_name
o22	0.00000	0.00000	0.00000	30.00	no_name

See file PEST_SOIL_CONCENTRATIONS.RES for more details of residuals in graph-ready format.

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See file PEST_SOIL_CONCENTRATIONS.SEO for composite observation sensitivities.

Objective function ----->

Sum of squared weighted residuals (ie phi) = 910.8

Correlation Coefficient ----->

Correlation coefficient = 0.9261

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	=	22
Mean value of non-zero weighted residuals	=	3.666
Maximum weighted residual [observation "o5"]	=	15.03
Minimum weighted residual [observation "o19"]	=	-6.389
Standard variance of weighted residuals	=	45.54
Standard error of weighted residuals	=	6.748

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.)
If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	6.1741E+05	-0.2037
kdeg	-0.2037	6.0053E-07

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	-0.3345
kdeg	-0.3345	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	-3.2992E-07	-1.000
kdeg	-1.000	3.2992E-07

Eigenvalues ----->

5.3330E-07 6.1741E+05

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	3676.00	2036.92	5315.08
DT50	2475.53	365.48	-518.62

Minimum error for which the Chi²-Test passes according to FOCUS: 69.50 %

4.11 Inverse modelling: Lindane, high dose, no weighting

PEST RUN RECORD: CASE PEST_SOIL_CONCENTRATIONS

PEST run mode:-

Parameter estimation mode

Case dimensions:-

Number of parameters	:	2
Number of adjustable parameters	:	2
Number of parameter groups	:	2
Number of observations	:	23
Number of prior estimates	:	0

Model command line(s):-

run_pesticide

Jacobian command line:-

na

Model interface files:-

Templates:

PESTICIDE.TPL

for model input files:

LINDANE_20000.PSM

(Parameter values written using single precision protocol.)

(Decimal point always included.)

Instruction files:

PEST.INS

for reading model output files:

PEST_SOIL.PLM

PEST-to-model message file:-

na

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central	Multiplier (central)	Method (central)
koc	relative	1.0000E-02	none	switch	2.000	parabolic
kdeg	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound
koc	none	relative	1200.00	100.000	1.000000E+06
kdeg	none	relative	2.670000E-03	2.700000E-04	2.666000E-02

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Name	Group	Scale	Offset	Model command number
koc	koc	1.00000	0.00000	1
kdeg	kdeg	1.00000	0.00000	1

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	61.5233	1.000	no_name
o2	0.158333	1.000	no_name
o3	0.00000	1.000	no_name
o4	44.1014	1.000	no_name
o5	3.87829	1.000	no_name
o6	0.331000	1.000	no_name
o7	8.450000E-02	1.000	no_name
o8	20.0764	1.000	no_name
o9	0.460571	1.000	no_name
o10	8.328571E-02	1.000	no_name
o11	5.657143E-02	1.000	no_name
o12	18.4383	1.000	no_name
o13	5.82400	1.000	no_name
o14	0.388571	1.000	no_name
o15	0.197000	1.000	no_name
o16	20.9584	1.000	no_name
o17	1.27286	1.000	no_name
o18	0.333000	1.000	no_name
o19	4.350000E-02	1.000	no_name
o20	12.9901	1.000	no_name
o21	3.18714	1.000	no_name
o22	0.336714	1.000	no_name
o23	0.00000	1.000	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

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OPTIMISATION RECORD

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 1743.5

Current parameter values

koc 1200.00
kdeg 2.670000E-03

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 1743.5

Lambda = 5.0000 ----->
Phi = 1367.7 (0.784 of starting phi)

Lambda = 2.5000 ----->
Phi = 1255.3 (0.720 of starting phi)

Lambda = 1.2500 ----->
Phi = 1137.5 (0.652 of starting phi)

Lambda = 0.62500 ----->
Phi = 1064.2 (0.610 of starting phi)

Lambda = 0.31250 ----->
Phi = 1037.0 (0.595 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 1037.0

Current parameter values

koc 3745.00
kdeg 2.700000E-04

Previous parameter values

koc 1200.00
kdeg 2.670000E-03

Maximum relative change: 2.121 ["koc"]

OPTIMISATION ITERATION NO. : 2
Model calls so far : 8
Starting phi for this iteration: 1037.0
parameter "kdeg" frozen: gradient and update vectors out of bounds

Lambda = 0.15625 ----->
Phi = 607.14 (0.585 of starting phi)

Lambda = 7.81250E-02 ----->
Phi = 607.14 (0.585 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 607.14

Current parameter values

koc 9614.00
kdeg 2.700000E-04

Previous parameter values

koc 3745.00
kdeg 2.700000E-04

Maximum relative change: 1.567 ["koc"]

OPTIMISATION ITERATION NO. : 3
Model calls so far : 12
Starting phi for this iteration: 607.14
All frozen parameters freed.

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```
Lambda = 7.81250E-02 ----->
Phi = 151.19 ( 0.249 of starting phi)
```

No more lambdas: phi is less than 0.3000 of starting phi
Lowest phi this iteration: 151.19

Current parameter values		Previous parameter values	
koc	25000.0	koc	9614.00
kdeg	4.500000E-04	kdeg	2.700000E-04
Maximum relative change: 1.600		["koc"]	

```
OPTIMISATION ITERATION NO.      :    4
Model calls so far              :   15
Starting phi for this iteration: 151.19
```

```
Lambda = 3.90625E-02 ----->
Phi = 129.51 ( 0.857 of starting phi)
```

```
Lambda = 1.95313E-02 ----->
Phi = 129.51 ( 0.857 of starting phi)
```

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 129.51

Current parameter values		Previous parameter values	
koc	31000.0	koc	25000.0
kdeg	2.700000E-04	kdeg	4.500000E-04
Maximum relative change: 0.4000		["kdeg"]	

```
OPTIMISATION ITERATION NO.      :    5
Model calls so far              :   19
Starting phi for this iteration: 129.51
parameter "kdeg" frozen: gradient and update vectors out of bounds
```

```
Lambda = 1.95313E-02 ----->
Phi = 129.49 ( 1.000 of starting phi)
```

```
Lambda = 9.76563E-03 ----->
Phi = 129.49 ( 1.000 of starting phi)
```

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 129.49
Relative phi reduction between optimisation iterations less than 0.1000
Switch to central derivatives calculation

Current parameter values		Previous parameter values	
koc	30000.0	koc	31000.0
kdeg	2.700000E-04	kdeg	2.700000E-04
Maximum relative change: 3.2258E-02		["koc"]	

```
OPTIMISATION ITERATION NO.      :    6
Model calls so far              :   23
Starting phi for this iteration: 129.49
All frozen parameters freed.
parameter "kdeg" frozen: gradient and update vectors out of bounds
```

```
Lambda = 9.76563E-03 ----->
Phi = 129.49 ( 1.000 times starting phi)
```

```
Lambda = 4.88281E-03 ----->
Phi = 129.49 ( 1.000 times starting phi)
```

No more lambdas: relative phi reduction between lambdas less than 0.0300

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Lowest phi this iteration: 129.49

Current parameter values		Previous parameter values	
koc	30000.0	koc	30000.0
kdeg	2.700000E-04	kdeg	2.700000E-04
Maximum relative change: 0.000		["koc"]	

Optimisation complete: the 3 lowest phi's are within a relative distance of each other of 1.000E-02

Total model calls: 27

The model has been run one final time using best parameters.
Thus all model input files contain best parameter values, and model output files contain model results based on these parameters.

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	30000.0	21944.3	38055.7
kdeg	2.700000E-04	-1.021323E-03	1.561323E-03

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in parameter space as the confidence limits themselves - see PEST manual.

See file PEST_SOIL_CONCENTRATIONS.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	61.5233	58.7760	2.74733	1.000	no_name
o2	0.158333	0.00000	0.158333	1.000	no_name
o3	0.00000	0.00000	0.00000	1.000	no_name
o4	44.1014	40.4270	3.67443	1.000	no_name
o5	3.87829	5.000000E-03	3.87329	1.000	no_name
o6	0.331000	0.00000	0.331000	1.000	no_name
o7	8.450000E-02	0.00000	8.450000E-02	1.000	no_name
o8	20.0764	24.3820	-4.30557	1.000	no_name
o9	0.460571	2.700000E-02	0.433571	1.000	no_name
o10	8.328571E-02	0.00000	8.328571E-02	1.000	no_name
o11	5.657143E-02	0.00000	5.657143E-02	1.000	no_name
o12	18.4383	16.8440	1.59429	1.000	no_name
o13	5.82400	8.600000E-02	5.73800	1.000	no_name
o14	0.388571	0.00000	0.388571	1.000	no_name
o15	0.197000	0.00000	0.197000	1.000	no_name
o16	20.9584	16.5440	4.41443	1.000	no_name
o17	1.27286	0.108000	1.16486	1.000	no_name
o18	0.333000	0.00000	0.333000	1.000	no_name
o19	4.350000E-02	0.00000	4.350000E-02	1.000	no_name
o20	12.9901	16.0240	-3.03386	1.000	no_name
o21	3.18714	0.249000	2.93814	1.000	no_name
o22	0.336714	0.00000	0.336714	1.000	no_name
o23	0.00000	0.00000	0.00000	1.000	no_name

See file PEST_SOIL_CONCENTRATIONS.RES for more details of residuals in graph-ready format.

See file PEST_SOIL_CONCENTRATIONS.SEO for composite observation sensitivities.

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Objective function ----->

Sum of squared weighted residuals (ie phi) = 129.5

Correlation Coefficient ----->

Correlation coefficient = 0.9901

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	=	23
Mean value of non-zero weighted residuals	=	0.9240
Maximum weighted residual [observation "o13"]	=	5.738
Minimum weighted residual [observation "o8"]	=	-4.306
Standard variance of weighted residuals	=	6.166
Standard error of weighted residuals	=	2.483

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	1.5000E+07	0.5060
kdeg	0.5060	3.8543E-07

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	0.2104
kdeg	0.2104	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	3.3734E-08	-1.000
kdeg	-1.000	-3.3734E-08

Eigenvalues ----->

3.6880E-07	1.5000E+07
------------	------------

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	30000.0	21944.3	38055.7
DT50	2567.21	443.95	-678.68

Minimum error for which the Chi²-Test passes according to FOCUS: 23.52 %

4.12 Inverse modelling: Lindane, high dose, data weighting

PEST RUN RECORD: CASE PEST_SOIL_CONCENTRATIONS

PEST run mode:-

Parameter estimation mode

Case dimensions:-

Number of parameters	:	2
Number of adjustable parameters	:	2
Number of parameter groups	:	2
Number of observations	:	23
Number of prior estimates	:	0

Model command line(s):-

run_pesticide

Jacobian command line:-

na

Model interface files:-

Templates:

PESTICIDE.TPL

for model input files:

LINDANE_20000.PSM

(Parameter values written using single precision protocol.)

(Decimal point always included.)

Instruction files:

PEST.INS

for reading model output files:

PEST_SOIL.PLM

PEST-to-model message file:-

na

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central	Multiplier (central)	Method (central)
koc	relative	1.0000E-02	none	switch	2.000	parabolic
kdeg	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound
koc	none	relative	1200.00	100.000	1.000000E+06
kdeg	none	relative	2.670000E-03	2.700000E-04	2.666000E-02

Name	Group	Scale	Offset	Model command number
------	-------	-------	--------	----------------------

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koc	koc	1.00000	0.00000	1
kdeg	kdeg	1.00000	0.00000	1

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	61.5233	1.000	no_name
o2	0.158333	30.00	no_name
o3	0.00000	60.00	no_name
o4	44.1014	1.000	no_name
o5	3.87829	30.00	no_name
o6	0.331000	60.00	no_name
o7	8.450000E-02	30.00	no_name
o8	20.0764	5.000	no_name
o9	0.460571	30.00	no_name
o10	8.328571E-02	60.00	no_name
o11	5.657143E-02	30.00	no_name
o12	18.4383	5.000	no_name
o13	5.82400	30.00	no_name
o14	0.388571	60.00	no_name
o15	0.197000	30.00	no_name
o16	20.9584	5.000	no_name
o17	1.27286	30.00	no_name
o18	0.333000	60.00	no_name
o19	4.350000E-02	30.00	no_name
o20	12.9901	5.000	no_name
o21	3.18714	30.00	no_name
o22	0.336714	60.00	no_name
o23	0.00000	30.00	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

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OPTIMISATION RECORD

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 34386.

Current parameter values

koc 1200.00

kdeg 2.670000E-03

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 34386.

Lambda = 5.0000 ----->
Phi = 31976. (0.930 of starting phi)

Lambda = 2.5000 ----->
Phi = 31960. (0.929 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300

Lowest phi this iteration: 31960.

Relative phi reduction between optimisation iterations less than 0.1000

Switch to central derivatives calculation

Current parameter values

koc 1236.00

kdeg 4.800000E-04

Maximum relative change: 0.8202 ["kdeg"]

Previous parameter values

koc 1200.00

kdeg 2.670000E-03

OPTIMISATION ITERATION NO. : 2
Model calls so far : 5
Starting phi for this iteration: 31960.

Lambda = 1.2500 ----->
Phi = 31789. (0.995 of starting phi)

Lambda = 0.62500 ----->
Phi = 31749. (0.993 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300

Lowest phi this iteration: 31749.

Current parameter values

koc 1293.00

kdeg 6.200000E-04

Maximum relative change: 0.2917 ["kdeg"]

Previous parameter values

koc 1236.00

kdeg 4.800000E-04

OPTIMISATION ITERATION NO. : 3
Model calls so far : 11
Starting phi for this iteration: 31749.

Lambda = 0.31250 ----->
Phi = 31679. (0.998 of starting phi)

Lambda = 0.15625 ----->
Phi = 31692. (0.998 of starting phi)

Lambda = 0.62500 ----->
Phi = 31682. (0.998 of starting phi)

No more lambdas: phi rising

Lowest phi this iteration: 31679.

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Current parameter values		Previous parameter values	
koc	1344.00	koc	1293.00
kdeg	5.300000E-04	kdeg	6.200000E-04
Maximum relative change: 0.1452 ["kdeg"]			

Optimisation complete: the 3 lowest phi's are within a relative distance of each other of 1.000E-02

Total model calls: 18

The model has been run one final time using best parameters.
Thus all model input files contain best parameter values, and model output files contain model results based on these parameters.

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	1344.00	319.260	2368.74
kdeg	5.300000E-04	-3.108946E-03	4.168946E-03

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in parameter space as the confidence limits themselves - see PEST manual.

See file PEST_SOIL_CONCENTRATIONS.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	61.5233	34.9500	26.5733	1.000	no_name
o2	0.158333	0.00000	0.158333	30.00	no_name
o3	0.00000	0.00000	0.00000	60.00	no_name
o4	44.1014	18.3220	25.7794	1.000	no_name
o5	3.87829	0.229000	3.64929	30.00	no_name
o6	0.331000	0.00000	0.331000	60.00	no_name
o7	8.450000E-02	0.00000	8.450000E-02	30.00	no_name
o8	20.0764	17.0140	3.06243	5.000	no_name
o9	0.460571	0.974000	-0.513429	30.00	no_name
o10	8.328571E-02	5.000000E-03	7.828571E-02	60.00	no_name
o11	5.657143E-02	0.00000	5.657143E-02	30.00	no_name
o12	18.4383	13.7250	4.71329	5.000	no_name
o13	5.82400	2.44900	3.37500	30.00	no_name
o14	0.388571	6.000000E-02	0.328571	60.00	no_name
o15	0.197000	0.00000	0.197000	30.00	no_name
o16	20.9584	12.7590	8.19943	5.000	no_name
o17	1.27286	2.84800	-1.57514	30.00	no_name
o18	0.333000	9.700000E-02	0.236000	60.00	no_name
o19	4.350000E-02	0.00000	4.350000E-02	30.00	no_name
o20	12.9901	8.82000	4.17014	5.000	no_name
o21	3.18714	4.51100	-1.32386	30.00	no_name
o22	0.336714	0.447000	-0.110286	60.00	no_name
o23	0.00000	0.00000	0.00000	30.00	no_name

See file PEST_SOIL_CONCENTRATIONS.RES for more details of residuals in graph-ready format.

See file PEST_SOIL_CONCENTRATIONS.SEO for composite observation sensitivities.

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Objective function ----->

Sum of squared weighted residuals (ie phi) = 3.1679E+04

Correlation Coefficient ----->

Correlation coefficient = 0.6977

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	=	23
Mean value of non-zero weighted residuals	=	14.32
Maximum weighted residual [observation "o5"]	=	109.5
Minimum weighted residual [observation "o17"]	=	-47.25
Standard variance of weighted residuals	=	1509.
Standard error of weighted residuals	=	38.84

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.)
If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	2.4272E+05	-0.6080
kdeg	-0.6080	3.0607E-06

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	-0.7054
kdeg	-0.7054	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	-2.5050E-06	-1.000
kdeg	-1.000	2.5050E-06

Eigenvalues ----->

1.5376E-06 2.4272E+05

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	1344.00	319.260	2368.74
DT50	1307.82	166.26	-222.95

Minimum error for which the Chi²-Test passes according to FOCUS: 80.47 %

4.13 Inverse modelling: Imidacloprid, low dose

PEST RUN RECORD: CASE PEST_SOIL_CONCENTRATIONS

PEST run mode:-

Parameter estimation mode

Case dimensions:-

Number of parameters	:	2
Number of adjustable parameters	:	2
Number of parameter groups	:	2
Number of observations	:	23
Number of prior estimates	:	0

Model command line(s):-

run_pesticide

Jacobian command line:-

na

Model interface files:-

Templates:

PESTICIDE.TPL

for model input files:

IMIDA_LOW.PSM

(Parameter values written using single precision protocol.)

(Decimal point always included.)

Instruction files:

PEST.INS

for reading model output files:

PEST_SOIL.PLM

PEST-to-model message file:-

na

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central	Multiplier (central)	Method (central)
koc	relative	1.0000E-02	none	switch	2.000	parabolic
kdeg	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound
koc	none	relative	223.000	22.3000	22000.0
kdeg	none	relative	6.680000E-03	6.700000E-04	6.678000E-02

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Name	Group	Scale	Offset	Model command number
koc	koc	1.00000	0.00000	1
kdeg	kdeg	1.00000	0.00000	1

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	2.08090	1.000	no_name
o2	0.265000	1.000	no_name
o3	0.00000	1.000	no_name
o4	3.51000	1.000	no_name
o5	0.120000	1.000	no_name
o6	3.000000E-02	1.000	no_name
o7	0.00000	1.000	no_name
o8	1.79820	1.000	no_name
o9	0.183800	1.000	no_name
o10	5.000000E-02	1.000	no_name
o11	0.00000	1.000	no_name
o12	0.303700	1.000	no_name
o13	0.215400	1.000	no_name
o14	0.00000	1.000	no_name
o15	0.00000	1.000	no_name
o16	0.492000	1.000	no_name
o17	0.108100	1.000	no_name
o18	3.000000E-02	1.000	no_name
o19	2.000000E-02	1.000	no_name
o20	0.204300	1.000	no_name
o21	0.140900	1.000	no_name
o22	0.00000	1.000	no_name
o23	0.00000	1.000	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

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OPTIMISATION RECORD

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 2.1821

Current parameter values

koc 223.000

kdeg 6.680000E-03

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 2.1821

Lambda = 5.0000 ----->
Phi = 2.0387 (0.934 of starting phi)

Lambda = 2.5000 ----->
Phi = 2.0121 (0.922 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300

Lowest phi this iteration: 2.0121

Relative phi reduction between optimisation iterations less than 0.1000

Switch to central derivatives calculation

Current parameter values

koc 254.800

kdeg 1.032000E-02

Maximum relative change: 0.5449

Previous parameter values

koc 223.000

kdeg 6.680000E-03

["kdeg"]

OPTIMISATION ITERATION NO. : 2
Model calls so far : 5
Starting phi for this iteration: 2.0121

Lambda = 1.2500 ----->
Phi = 1.9236 (0.956 of starting phi)

Lambda = 0.6250 ----->
Phi = 1.8990 (0.944 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300

Lowest phi this iteration: 1.8990

Current parameter values

koc 364.600

kdeg 9.180000E-03

Maximum relative change: 0.4309

Previous parameter values

koc 254.800

kdeg 1.032000E-02

["koc"]

OPTIMISATION ITERATION NO. : 3
Model calls so far : 11
Starting phi for this iteration: 1.8990

Lambda = 0.31250 ----->
Phi = 1.8756 (0.988 of starting phi)

Lambda = 0.15625 ----->
Phi = 1.8773 (0.989 of starting phi)

Lambda = 0.62500 ----->
Phi = 1.8757 (0.988 of starting phi)

No more lambdas: phi rising

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Lowest phi this iteration: 1.8756

Current parameter values		Previous parameter values	
koc	399.600	koc	364.600
kdeg	1.016000E-02	kdeg	9.180000E-03
Maximum relative change: 0.1068		["kdeg"]	

OPTIMISATION ITERATION NO. : 4
Model calls so far : 18
Starting phi for this iteration: 1.8756

Lambda = 0.31250 ----->
Phi = 1.8740 (0.999 of starting phi)

Lambda = 0.15625 ----->
Phi = 1.8718 (0.998 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 1.8718

Current parameter values		Previous parameter values	
koc	497.300	koc	399.600
kdeg	1.061000E-02	kdeg	1.016000E-02
Maximum relative change: 0.2445		["koc"]	

OPTIMISATION ITERATION NO. : 5
Model calls so far : 24
Starting phi for this iteration: 1.8718

Lambda = 7.81250E-02 ----->
Phi = 1.8735 (1.001 times starting phi)

Lambda = 3.90625E-02 ----->
Phi = 1.8735 (1.001 times starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 1.8735

Current parameter values		Previous parameter values	
koc	497.100	koc	497.300
kdeg	1.078000E-02	kdeg	1.061000E-02
Maximum relative change: 1.6023E-02		["kdeg"]	

Optimisation complete: the 3 lowest phi's are within a relative distance
of eachother of 1.000E-02

Total model calls: 30

The model has been run one final time using best parameters.
Thus all model input files contain best parameter values, and model
output files contain model results based on these parameters.

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	497.300	1.53789	993.062
kdeg	1.061000E-02	5.240807E-03	1.597919E-02

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in

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parameter space as the confidence limits themselves - see PEST manual.

See file PEST_SOIL_CONCENTRATIONS.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	2.08090	2.65800	-0.577100	1.000	no_name
o2	0.265000	0.00000	0.265000	1.000	no_name
o3	0.00000	0.00000	0.00000	1.000	no_name
o4	3.51000	2.36900	1.14100	1.000	no_name
o5	0.120000	4.200000E-02	7.800000E-02	1.000	no_name
o6	3.000000E-02	0.00000	3.000000E-02	1.000	no_name
o7	0.00000	0.00000	0.00000	1.000	no_name
o8	1.79820	1.78200	1.620000E-02	1.000	no_name
o9	0.183800	0.163000	2.080000E-02	1.000	no_name
o10	5.000000E-02	1.000000E-03	4.900000E-02	1.000	no_name
o11	0.00000	0.00000	0.00000	1.000	no_name
o12	0.303700	0.689000	-0.385300	1.000	no_name
o13	0.215400	0.181000	3.440000E-02	1.000	no_name
o14	0.00000	5.000000E-03	-5.000000E-03	1.000	no_name
o15	0.00000	0.00000	0.00000	1.000	no_name
o16	0.492000	0.519000	-2.700000E-02	1.000	no_name
o17	0.108100	0.164000	-5.590000E-02	1.000	no_name
o18	3.000000E-02	7.000000E-03	2.300000E-02	1.000	no_name
o19	2.000000E-02	0.00000	2.000000E-02	1.000	no_name
o20	0.204300	0.246000	-4.170000E-02	1.000	no_name
o21	0.140900	0.149000	-8.100000E-03	1.000	no_name
o22	0.00000	1.800000E-02	-1.800000E-02	1.000	no_name
o23	0.00000	0.00000	0.00000	1.000	no_name

See file PEST_SOIL_CONCENTRATIONS.RES for more details of residuals in graph-ready format.

See file PEST_SOIL_CONCENTRATIONS.SEO for composite observation sensitivities.

Objective function ----->

Sum of squared weighted residuals (ie phi) = 1.872

Correlation Coefficient ----->

Correlation coefficient = 0.9431

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	=	23
Mean value of non-zero weighted residuals	=	2.4317E-02
Maximum weighted residual [observation "o4"]	=	1.141
Minimum weighted residual [observation "o1"]	=	-0.5771
Standard variance of weighted residuals	=	8.9134E-02
Standard error of weighted residuals	=	0.2986

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	5.6809E+04	0.3249
kdeg	0.3249	6.6633E-06

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	0.5281
kdeg	0.5281	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	5.7193E-06	-1.000
kdeg	-1.000	-5.7193E-06

Eigenvalues ----->

4.8050E-06 5.6809E+04

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	497.300	1.53789	993.062
DT50	65.33	43.38	132.26

Minimum error for which the Chi²-Test passes according to FOCUS: 57.63 %

4.14 Inverse modelling: Imidacloprid, high dose

PEST RUN RECORD: CASE PEST_SOIL_CONCENTRATIONS

PEST run mode:-

Parameter estimation mode

Case dimensions:-

Number of parameters	:	2
Number of adjustable parameters	:	2
Number of parameter groups	:	2
Number of observations	:	23
Number of prior estimates	:	0

Model command line(s):-

run_pesticide

Jacobian command line:-

na

Model interface files:-

Templates:

PESTICIDE.TPL

for model input files:

IMIDA_HIGH.PSM

(Parameter values written using single precision protocol.)

(Decimal point always included.)

Instruction files:

PEST.INS

for reading model output files:

PEST_SOIL.PLM

PEST-to-model message file:-

na

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central switch	Multiplier (central)	Method (central)
koc	relative	1.0000E-02	none	switch	2.000	parabolic
kdeg	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound
koc	none	relative	223.000	22.3000	22000.0
kdeg	none	relative	6.680000E-03	6.700000E-04	6.678000E-02

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Name	Group	Scale	Offset	Model command number
koc	koc	1.00000	0.00000	1
kdeg	kdeg	1.00000	0.00000	1

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	9.06000	1.000	no_name
o2	0.278301	1.000	no_name
o3	0.00000	1.000	no_name
o4	5.73000	1.000	no_name
o5	0.520000	1.000	no_name
o6	4.700000E-02	1.000	no_name
o7	0.00000	1.000	no_name
o8	4.18000	1.000	no_name
o9	1.15000	1.000	no_name
o10	0.120000	1.000	no_name
o11	0.00000	1.000	no_name
o12	0.580000	1.000	no_name
o13	0.210000	1.000	no_name
o14	3.300000E-02	1.000	no_name
o15	0.00000	1.000	no_name
o16	1.19000	1.000	no_name
o17	0.350000	1.000	no_name
o18	6.800000E-02	1.000	no_name
o19	0.00000	1.000	no_name
o20	0.750000	1.000	no_name
o21	0.490000	1.000	no_name
o22	7.900000E-02	1.000	no_name
o23	0.00000	1.000	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

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OPTIMISATION RECORD

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 10.949

Current parameter values

koc 223.000
kdeg 6.680000E-03

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 10.949

Lambda = 5.0000 ----->
Phi = 3.4732 (0.317 of starting phi)

Lambda = 2.5000 ----->
Phi = 3.4681 (0.317 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 3.4681

Current parameter values

koc 227.500
kdeg 1.265000E-02

Previous parameter values

koc 223.000
kdeg 6.680000E-03

Maximum relative change: 0.8937 ["kdeg"]

OPTIMISATION ITERATION NO. : 2
Model calls so far : 5
Starting phi for this iteration: 3.4681

Lambda = 1.2500 ----->
Phi = 2.8543 (0.823 of starting phi)

Lambda = 0.6250 ----->
Phi = 2.8474 (0.821 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 2.8474

Current parameter values

koc 245.900
kdeg 1.574000E-02

Previous parameter values

koc 227.500
kdeg 1.265000E-02

Maximum relative change: 0.2443 ["kdeg"]

OPTIMISATION ITERATION NO. : 3
Model calls so far : 9
Starting phi for this iteration: 2.8474

Lambda = 0.31250 ----->
Phi = 2.8444 (0.999 of starting phi)

Lambda = 0.15625 ----->
Phi = 2.8430 (0.998 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0300
Lowest phi this iteration: 2.8430
Relative phi reduction between optimisation iterations less than 0.1000
Switch to central derivatives calculation

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Current parameter values		Previous parameter values	
koc	243.900	koc	245.900
kdeg	1.596000E-02	kdeg	1.574000E-02

Maximum relative change: 1.3977E-02 ["kdeg"]

OPTIMISATION ITERATION NO. : 4
 Model calls so far : 13
 Starting phi for this iteration: 2.8430

Lambda = 7.81250E-02 ----->
 Phi = 2.8351 (0.997 of starting phi)

Lambda = 3.90625E-02 ----->
 Phi = 2.8353 (0.997 of starting phi)

Lambda = 0.15625 ----->
 Phi = 2.8384 (0.998 of starting phi)

No more lambdas: phi rising
 Lowest phi this iteration: 2.8351

Current parameter values		Previous parameter values	
koc	257.800	koc	243.900
kdeg	1.637000E-02	kdeg	1.596000E-02

Maximum relative change: 5.6991E-02 ["koc"]

Optimisation complete: the 3 lowest phi's are within a relative distance
 of eachother of 1.000E-02
 Total model calls: 20

The model has been run one final time using best parameters.
 Thus all model input files contain best parameter values, and model
 output files contain model results based on these parameters.

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	257.800	147.745	367.855
kdeg	1.637000E-02	1.249444E-02	2.024556E-02

Note: confidence limits provide only an indication of parameter uncertainty.
 They rely on a linearity assumption which may not extend as far in
 parameter space as the confidence limits themselves - see PEST manual.

See file PEST_SOIL_CONCENTRATIONS.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	9.06000	8.20100	0.859000	1.000	no_name
o2	0.278301	0.00000	0.278301	1.000	no_name
o3	0.00000	0.00000	0.00000	1.000	no_name
o4	5.73000	6.65300	-0.923000	1.000	no_name
o5	0.520000	0.396000	0.124000	1.000	no_name
o6	4.700000E-02	1.000000E-03	4.600000E-02	1.000	no_name
o7	0.00000	0.00000	0.00000	1.000	no_name
o8	4.18000	3.94300	0.237000	1.000	no_name
o9	1.15000	1.08800	6.200000E-02	1.000	no_name

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o10	0.120000	2.400000E-02	9.600000E-02	1.000	no_name
o11	0.000000	0.000000	0.000000	1.000	no_name
o12	0.580000	0.816000	-0.236000	1.000	no_name
o13	0.210000	0.567000	-0.357000	1.000	no_name
o14	3.300000E-02	6.200000E-02	-2.900000E-02	1.000	no_name
o15	0.000000	0.000000	0.000000	1.000	no_name
o16	1.190000	0.518000	0.672000	1.000	no_name
o17	0.350000	0.411000	-6.100000E-02	1.000	no_name
o18	6.800000E-02	6.100000E-02	7.000000E-03	1.000	no_name
o19	0.000000	0.000000	0.000000	1.000	no_name
o20	0.750000	0.159000	0.591000	1.000	no_name
o21	0.490000	0.186000	0.304000	1.000	no_name
o22	7.900000E-02	6.800000E-02	1.100000E-02	1.000	no_name
o23	0.000000	0.000000	0.000000	1.000	no_name

See file PEST_SOIL_CONCENTRATIONS.RES for more details of residuals in graph-ready format.

See file PEST_SOIL_CONCENTRATIONS.SEO for composite observation sensitivities.

Objective function ----->

Sum of squared weighted residuals (ie phi) = 2.835

Correlation Coefficient ----->

Correlation coefficient = 0.9876

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	=	23
Mean value of non-zero weighted residuals	=	7.3100E-02
Maximum weighted residual [observation "o1"]	=	0.8590
Minimum weighted residual [observation "o4"]	=	-0.9230
Standard variance of weighted residuals	=	0.1350
Standard error of weighted residuals	=	0.3674

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	2800.	4.5995E-02
kdeg	4.5995E-02	3.4717E-06

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	0.4665
kdeg	0.4665	1.000

Normalized eigenvectors of parameter covariance matrix ----->

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	Vector_1	Vector_2
koc	1.6429E-05	-1.000
kdeg	-1.000	-1.6429E-05

Eigenvalues ----->

2.7160E-06 2800.

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
koc	257.800	147.745	367.855
DT50	42.34	34.24	55.48

Minimum error for which the Chi²-Test passes according to FOCUS: 27.28 %