Supporting Information

NON-EXTRACTABLE RESIDUES (NER) IN PERSISTENCE ASSESSMENT – EFFECT ON THE DEGRADATION HALF-LIFE OF CHEMICALS

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Table of Contents

Details on the fit procedure

Recovery: OECD 307, 308 and 309 says that recovery should be 90-110%. Not accepted in our study if minimum recovery is <70% or the recovery vary more than 30 % (pyriproxyfen OECD 308 excluded).

Time zero values: Adding NER and metabolite measured to parent and setting NER/metabolite value to 0 for parent scenario (all scenarios for metabolite). When the first measurement occurred later than day 0 (at day 1 or 7), a day 0 point was added as the average recovery for the test as parent. NER, metabolite and CO_2 was set to 0. This was done as M0 for parent should be around 100% when just added, however, in some studies the recoveries in the study never reached 100 % (e.g. 93 % in average) and therefore just choosing 100 % when the method had a lower recovery, would make the added M0 artificially high. This was done for bromoxynil in Possberg et al. (2016) which had the first measured point at day 7 and for C-DA+, C-DP, C-DS- and deltamethrin, which all had first measured point at day 1. The resulting changes were small for all cases where the first measurement was at day 1. For Possberg however, the change was significant, as the assumed starting value varied greatly otherwise. As an example in scenario i in Possberg, predicted value with an SFO fit was around 14, and for scenario ii with DFOP M0 was predicted to be around 1400. Therefore, we would have to fix a starting value anyway to be able to use the data from Possberg. In scenario iv for bromoxynil (UBA) NER I was not measured with silylation until day 7 and for isoproturon (UBA) first measurement of NER I for

both silylation and EDTA was at day 7. Therefore a point 0 was added, assuming no NER I formed on day 0. This resulted in small changes compared to not adding a point at time 0.

For 5 compounds (2,4-D, bromoxynil, C-DA+, fenoxycarb and triclosan, there were scenarios where the predicted and measured M0 were far apart (<20%) in the SFO fit and it was investigated if the fit could be improved by fixing M0. In all cases, the predicted value was lower than the measured value, and these curves typically stagnated. For all cases we found that the DegT50 value found without fixing M0 were more representative than when fixing the value, and therefore we chose not to fix any starting values.

Matabolite fit: Metabolites for glyphosate, thiamethoxam and triclosan. The amount of metabolite is the same in all scenarios, as their only difference is approach towards NER. For all substances, the metabolite kinetic was chosen to be SFO, as DFOP kinetics for the metabolite didn't lead to an improvement but added unnecessary complexity and long running times in CAKE. SFO described the metabolites sufficiently. The big change for the metabolite curve was seen in the choice of parent kinetic, and often improved when DFOP was chosen.

Lag phase: Metamitron might have a lag phase, but there are too few data points to see if it is. Otherwise, no lag phases in data sets.

Outliers: In most of the studies, there are too few datapoints to detect actual outliers. In the cases where some values looked unlikely (e.g. parent rising in the middle of experiment to a value higher than measured at time 0), these were due to studies with poor recovery or a high variation in recovery.

<LOD / LOQ: no LOD or LOQ stated in any of the studies, so we could not add a point where we take half of LOD or LOQ. We tried adding a point 0 in the end as first point with measurements < LOD or LOQ but that changed the DegT50 quite a bit, so decided to just leave these points out

308 and 309 tests: Made DegT50 values for entire system, not divided into environmental matrix

MTB bioNER > total NER: When calculated MTBbioNER is higher than measured total NER, MTBbioNER is set to be equal to total NER, so we don't make illogical calculations for scenario iii.

SI Table 1. Goodness-of-fit statistics and calibrated half-lives with single first-order (SFO) and Double-First-Order in Parallel (DFOP) kinetics. t-test is passed P for P < 0.05, else not passed NP.

Substance	**Scen.**	**Visual**		**X^2**		**t-test**		**DegT50**		
		SFO	DFOP	SFO	DFOP	SFO	DFOP	SFO	DFOP (overall)	DFOP (slow phase)
2,4-D	i	Good	Good, but not actually biphasic, so SFO better	22.8	27.2	NP	P NP	2.81	2.81	>10000
	ii	Not acceptable – definitely biphasic!	Good	28.5	15.9	NP	NP NP	42.7	5.28	>10000
	iii	Not acceptable – definitely biphasic!	Good	29.6	18.4	P	NP NP	5.88	4.06	>10000
Acetaminophen	A i	Miss all after point 3	Good	20.5	4.05	NP	P NP	0.484	0.451	1560
	A ii	Fine – equally good	Fine – equally good	2.77	2.47	P	NP P	792	945	1050
	A iii	Fine – equally good	Fine – equally good	3.22	2.5	P	NP P	490	542	630
	B i	Not acceptable – definitely biphasic!	Good	44.3	13.1	P	P NP	1.58	1.17	160
	B ii	Fine – equally good	Fine – equally good	1.76	1.93	P	N/A P	714	714	715
	B iii	Fine – equally good	Fine – equally good	1.8	1.79	P	NP P	539	549	578
	C i	Miss all after point 3	Good	25.8	1.76	P	P P	0.498	0.438	221
	C ii	Fine – equally good	Fine – equally good	2.31	1.59	P	NP P	616	714	806
	C iii	Fine – equally good	Fine – equally good	2.84	1.73	P	NP P	439	478	559

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Atrazine	i	Good	Good	1.57	0.89	P	NP NP	211	>10000	>10000
	ii	Good	Good	1.2	1.5	NP	NP NP	>10000	>10000	>10000
	iii	Good	Good	1.07	1.35	NP	NP NP	>10000	>10000	>10000
Benzovindiflupyr	i	Biphasic, so DFOP better	Good	6.41	4.14	NP	NP NP	322	774	1140
	ii	Biphasic	Good	6.09	4.35	NP	NP NP	649	>10000	>10000
	iii	Biphasic	Good	6.1	4.31	NP	NP NP	621	>10000	>10000
Bromoxynil UBA	i	OK	Good	7.72	3.38	P	P P	8.09	6.57	10.1
	ii	Poor - biphasic	Good	6.7	1.36	P	P P	154	260	415
	iii	Poor - biphasic	Good	6.85	1.25	P	P P	130	187	301
	iv sily	OK	Good	10.9	0.673	P	P NP	13	10.6	167
	iv EDTA	Not great	Good	13.5	1.66	P	P NP	14.5	10.6	143
Bromoxynil Possberg	i	OK	Good	11.4	1.39	P	P NP	2.56	2.12	113
	ii	Not great, not terrible	Good	4.52	2.01	NP	NP NP	216	1210	1670
	iii	Not great, not terrible	Good	5.14	2.05	NP	NP NP	180	770	1120
C-DA+	308 i	Not acceptable - biphasic	Good	14	2.3	P	P P	108	74.8	230
	308 ii	Good	Good	2.43	2.72	P	NP NP	457	503	525

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
C-DA+	308 iii	Good	Good	2.52	2.71	P	NP P	355	386	410
	309 i	Not good	OK	9.04	2.84	NP	NP NP	375	>10000	>10000
	309 ii	OK	OK	1.48	0.613	P	NP NP	524	>10000	>10000
	309 iii	OK	OK	2.02	0.433	P	NP NP	306	>10000	>10000
C-DP	308 i	Good	Good	11.1	12.3	P	NP NP	10.4	9.93	118
	308 ii	Okay	Okay (last point better described)	9.56	8.36	P	NP NP	27.6	23	222
	308 iii	Good	Good	10.7	12.4	P	NP NP	12.1	11.8	>10000
	309 i	Good	Good	6.98	7.38	P	NP NP	17.6	16	>10000
	309 ii	Good	Good	5.85	4.78	P	NP NP	36.6	31.9	>10000
	309 iii	Good	Good	6.57	6.9	P	NP NP	17.5	16.1	>10000
C-DS-	308 i	Good	Good	9	10.7	P	NP NP	12.9	12.8	>10000
	308 ii	Good	Good	7.3	6.61	P	NP NP	36.4	31.7	>10000
	308 iii	Good	Good	8.55	10.2	P	P P	17.9	17.9	17.9
	309 i	Good	Good	6.94	5.95	P	NP NP	21.4	18.4	>10000
	309 ii	Good	Good	5.15	5.22	P	NP NP	30.8	27.9	>10000
	309 iii	Good	Good	7.38	6.56	P	NP NP	21.1	18	>10000

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Celecoxib	308 We i	OK	OK	3.94	4.54	NP	NP NP	1870	1870	1880
	308 We ii	OK	OK	4.27	4.92	NP	NP NP	>10000	>10000	>10000
	308 We iii	OK	OK	4.34	5	NP	NP NP	>10000	>10000	>10000
	308 Wi i	OK	OK	6.11	7.04	NP	NP NP	5850	5850	5870
	308 Wi ii	OK	OK	7.13	8.22	NP	NP NP	>10000	>10000	>10000
	308 Wi iii	OK	OK	7.15	8.24	NP	NP NP	>10000	>10000	>10000
	309 We i	Fair	Good	8.51	4.17	P	NP NP	59.4	>10000	>10000
	309 We ii	Good	Good	2.79	2.71	NP	NP NP	641	>10000	>10000
	309 We iii	Good	Good	2.84	2.72	NP	NP NP	600	>10000	>10000
	309 Wi i	Fair	Good	5.18	2.13	P	NP P	125	148	204
	309 Wi ii	Good	Good	2.28	0.944	P	NP NP	503	>10000	>10000
	309 Wi iii	Good	Good	2.33	0.958	P	NP NP	478	>10000	>10000
Ciprofloxacin	i	Not acceptable	Good	21.6	0.0452	P	P P	11.4	6.6	111
	ii	Good	Good	2.16	3.08	NP	NP NP	>10000	>10000	>10000
	iii	Good	Good	1.99	2.84	NP	NP NP	>10000	>10000	>10000

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Deltamethin	CLS i	Good	Good	2.1	2.42	P	NP NP	137	159	>10000
	CLS ii	Good	Good	1.83	2.17	P	NP NP	222	257	>10000
	CLS iii	Good	Good	1.99	2.32	P	NP P	178	234	>10000
	SC i	Good	Good	3.54	4.21	P	NP NP	144	144	144
	SC ii	Good	Good	2.97	3.54	P	NP NP	266	323	>10000
	SC iii	Good	Good	3.08	3.67	P	NP NP	221	221	221
Dicamba	i	Good	Good	7.99	8.71	P	P NP	9.42	9.18	>10000
	ii	Good	Good	3.94	4.07	P	NP NP	189	>10000	>10000
	iii	Good	Good	4.75	4.59	P	NP NP	137	>10000	>10000
Fenoxycarb	2.2 i	Only describes first 2 points, but the rest is only a few %	Good	11.8	1.5	P	NP NP	2.7	1.07	136
	2.2 ii	Bad – not acceptable	Good	17.9	2.26	P	NP NP	95.4	72.9	1420
	2.2 iii	Bad – not acceptable	Good	28.3	5.23	NP	NP NP	35.4	7.54	436
	2.2 iv	Not good	Good	19.1	2.23	P	NP NP	3.28	0.408	181
	2.3 i	OK - only describes first 2 points, but the rest is < 5 %	Good	11.6	0.679	P	P NP	3.07	2.52	>10000
	2.3 ii	Bad – not acceptable	Good	11.2	1.42	P	NP NP	112	665	3350

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Fenoxycarb	2.3 iii	Bad – not acceptable	Good	16.9	2.32	P	NP NP	52.3	20	1530
	2.3 iv	Not good	Good	23.1	2.92	P	NP NP	4.36	3.23	>10000
	2.4 i	Only describes first 2 points, but the rest is only a few %	Good	12.6	0.971	P	NP NP	2.8	0.374	105
	2.4 ii	Bad – not acceptable	Good	12.4	0.0811	NP	P P	135	244	696
	2.4 iii	Bad – not acceptable	Good	19.8	0.271	NP	P P	65.1	14.3	319
	2.4 iv	Not good	Good	18.2	2.21	P	NP NP	3.69	2.25	116
Glyphosate AMPA	i	OK – difficult case with the metabolite as CAKE can't describe cases with "lag phase" for metabolites well	OK, same issues as with SFO	10 16.6	8.84 17.1	P NP	NP P NP	14.3 >10000	12.5 >10000	16.4 N/A
	ii	Good	Good	5.7 9	7.11 10.1	P NP	NP NP P	37.2 >10000	36.9 >10000	>10000 N/A
	iii	OK	OK	10.4 15.2	13.1 17.1	P NP	NP NP NP	23.2 >10000	23.1 >10000	>10000 N/A
Ibuprofen	i	Good	Good	4.7	5.59	P	P N/A	10.8	10.8	43.9
	ii	Acceptable, although it looks like it could be biphasic	Good	8.68	3.48	P	NP NP	46	30.7	>10000
	iii	Good	Good	4.77	5.22	P	NP NP	20.3	19.5	>10000

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Isoproturon UBA	i	Good	Good	3.42	3.69	P	NP NP	53.6	52.7	57.3
	ii	OK, but might be biphasic	Good	3.55	2.68	P	NP P	263	362	478
	iii	Good	Good	3.46	3	P	NP P	168	181	230
	iv sily	Good	Good	3.74	2.9	P	NP P	68.4	63.4	94.7
	iv EDTA	Good	Good	3.16	2.47	P	NP P	67.3	63.2	88.3
Isoproturon Mordaunt	i	OK	Better	9.9	8.1	P	NP NP	21.7	18.8	>10000
	ii	OK	Good	4.14	3.57	P	NP NP	186	>10000	>10000
	iii	OK	Good	6.09	5.39	P	NP NP	105	>10000	>10000
Lindane	i	Good	Good	1.79	0.638	P	NP NP	238	>10000	>10000
	ii	Good	Good	1.28	0.339	P	NP P	401	588	654
	iii	Good	Good	1.18	0.358	P	NP P	332	410	447
Metamitron	i	OK	OK (but not biphasic, g=1)	23.3	33.3	P	NP N/A	4.09	4.09	35.7
	ii	OK	OK	12	12.8	P	NP NP	13	10.4	>10000
	iii	OK	OK	14	19.8	P	NP NP	7.6	7.46	>10000
Pyriproxyfen (parent + metabolite pool)	We i	OK – what is wrong is not the curve, more the scatter	OK – but scatter	8.42	9.41	P	NP NP	124	136	156

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Pyriproxyfen (parent + metabolite pool)	We ii	OK	OK	6.14	7.07	NP	NP NP	1930	3020	3070
	We iii	OK	OK	6.13	7.05	NP	NP NP	607	709	725
	Wi i	OK – recovery is not good. Average is around 80%. Making the data unreliable	OK – recovery is not good, around 80%, making the data unreliable	6.8	6.57	P	NP NP	92.5	242	459
	Wi ii	OK	OK	5.52	6.03	P	NP NP	227	>10000	>10000
	Wi iii	OK	OK	5.43	6.07	P	NP NP	173	>10000	>10000
Sulfadiazine	i	OK, but M0 and the last datapoints are not well described	Good	9.34	4.12	P	P P	10.1	6.99	22.1
	ii	OK	OK	2.7	3.03	NP	NP NP	>10000	>10000	>10000
	iii	OK	OK	2.7	3.03	NP	NP NP	>10000	>10000	>10000
	iv EDTA	Not great	Good	10.6	0.154	P	P P	37.4	25.3	151
Thiamethoxam (Clothianidine)	GAR i	Good	Good	4.56 5.72	5.15 6.13	P NP	P P NP	33.5 >10000	33.5 >10000	33.5 N/A
	GAR ii	Good	Good	2.6 3.44	2.78 3.5	P NP	NP NP NP	51.9 404	50.1 990	>10000 N/A
	GAR iii	Good	Good	4.69 5.9	5.27 6.31	P NP	P nd NP	33.5 >10000	33.3 >10000	33.5 N/A
	18A i	Looks (slightly) biphasic, but acceptable	Good	4.74 6.41	2.42 3.28	P NP	P P NP	140 74.7	177 >10000	283 N/A

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Thiamethoxam (Clothianidine)	18A ii	Looks (slightly) biphasic, but acceptable	Good	5.93 8.02	2.7 3.7	P NP	P NP NP	173 65.6	>10000 >10000	>10000 N/A
	18A iii	Looks (slightly) biphasic, but acceptable	Good	6.1 8.24	2.44 3.37	P NP	P NP NP	142 74.2	>10000 >10000	>10000 N/A
	EAS i	OK	Good	3.65 5.02	2.69 3.92	P P	NP P NP	61 198	56.7 >10000	73.7 N/A
	EAS ii	OK	Good	3.25 4.54	2.79 3.93	P P	NP NP NP	63.3 183	57.9 1290	226 N/A
	EAS iii	OK	Good	3.49 4.82	2.56 3.72	P NP	P NP NP	57.7 225	51.2 >10000	>10000 N/A
	SAR i	Looks (slightly) biphasic, but acceptable	Good	5.93 7.63	3.28 4.36	P P	P NP NP	89 50.3	82 679	438 N/A
	SAR ii	Looks (slightly) biphasic, but acceptable	Good	4.76 6.2	3.75 4.87	P P	NP NP NP	97.5 47.1	99.4 183	200 N/A
	SAR iii	Looks (slightly) biphasic, but acceptable	Good	5.77 7.44	3.48 4.56	P P	P NP NP	88.8 50.4	82.1 473	527 N/A
Triclosan (Methyl-triclosan)	2.2 i	Okay	Good	8.12 10.9	0.525 4.66	P NP	P P NP	54.1 >10000	43.7 >10000	71.5 N/A
	2.2. ii	Good	Good	2.42 3.85	1.21 2.51	P NP	NP P NP	152 161	158 >10000	180 N/A
	2.2 iii	Good	Good	2.51 3.97	1.23 2.54	P NP	NP P NP	139 178	144 >10000	166 N/A

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Triclosan (Methyl-triclosan)	2.2 iv	Good	Good	1.43 3.26	0.371 3.07	P NP	NP P NP	70.7 >10000	69.6 >10000	85.1 N/A
	2.3 i	Only first two points well described, hereafter few % left	Good	11.8 14.2	2.63 6.99	P NP	P NP NP	3.42 >10000	2.9 >10000	48.4 N/A
	2.3 ii	Okay	Good	7.9 11.1	3.49 4.03	P NP	NP NP NP	119 31.5	159 >10000	273 N/A
	2.3 iii	Okay	Good	8.1 11.3	3.63 4.19	P NP	NP P NP	108 28.6	120 1170	212 N/A
	2.3 iv	Not good	Good	28.3 34.1	4.4 6.6	P NP	P NP NP	5.31 >10000	3.85 >10000	162 N/A
	2.4 i	Good	Good	11.7 9.29	0.255 9.37	P P	P P P	4.89 83.2	4.07 95.6	55.9 N/A
	2.4 ii	Horrible fit	Good	45.1 39.2	16.7 12.9	P P	P NP NP	5.93 70.4	8.52 84.9	>10000 N/A
	2.4 iii	Horrible fit	Good	42.1 35.8	9.28 9.25	P P	P NP NP	5.97 69.8	6.56 103	>10000 N/A
	2.4 iv	OK	Good	15.7 11.2	0.0292 7.29	P P	P P P	5.75 72.9	5.21 82.8	113 N/A
Trifluralin	i	Good	Good	2.05	1.55	P	NP NP	175	279	410
	ii	Good	Good	1.08	1.36	P	NP NP	656	665	666
	iii	Good	Good	1.12	1.4	P	N/A P	570	570	568

Substance	Scen.	Visual - SFO	Visual DFOP	X^2 SFO	X^2 DFOP	t-test	t-test	DegT50 SFO	DFOP overall	DFOP slow
Voriconazole	308 We i	Good	Good	0.85	0.533	P	NP P	249	269	281
	308 We ii	Good	Good	1.05	0.841	P	NP P	442	529	555
	308 We iii	Good	Good	1.11	0.883	P	NP P	418	502	529
	308 Wi i	Good	Good	1.79	1.91	P	NP NP	216	>10000	>10000
	308 Wi ii	Good	Good	1.73	1.99	NP	NP P	977	977	976
	308 Wi iii	Good	Good	1.71	1.96	NP	P NP	901	901	903
	309 We i	Good	Good	2.53	2.49	P	NP NP	203	>10000	>10000
	309 We ii	Good	Good	2.28	2.62	NP	N/A NP	>10000	>10000	>10000
	309 We iii	Good	Good	2.43	2.8	NP	NP NP	>10000	>10000	>10000
	309 Wi i	Good	Good	2.56	2.95	NP	N/A NP	>10000	>10000	>10000
	309 Wi ii	Good	Good	3.04	3.5	NP	N/A NP	>10000	>10000	>10000
	309 Wi iii	Good	Good	2.97	3.42	NP	N/A NP	>10000	>10000	>10000

For substances with metabolites (glyphosate, thiamethoxam and triclosan), the χ^2 stated is for parent followed by for overall system, t-test is for parent k (for DFOP this is two values) followed by metabolite k. DegT50 is for parent first, then metabolite.

t-test: P is passed ($P < 0.05$), NP is not passed, N/A is not applicable, nd is not determined. In t-test DFOP, first notation is for the fast degradation rate, the second is for slow degradation rate

A, B, C, SAR, GAR, 18A, EAS, We, Wi, 2.2, 2.3, 2.4 denote tests in different soils.

308 and 309 denote tests in sediment (OECD 308) or surface water (OECD 309). All other tests were in soil (OECD 307 or similar).