Challenges in kinetic analyses of pesticide degradation and dissipation studies

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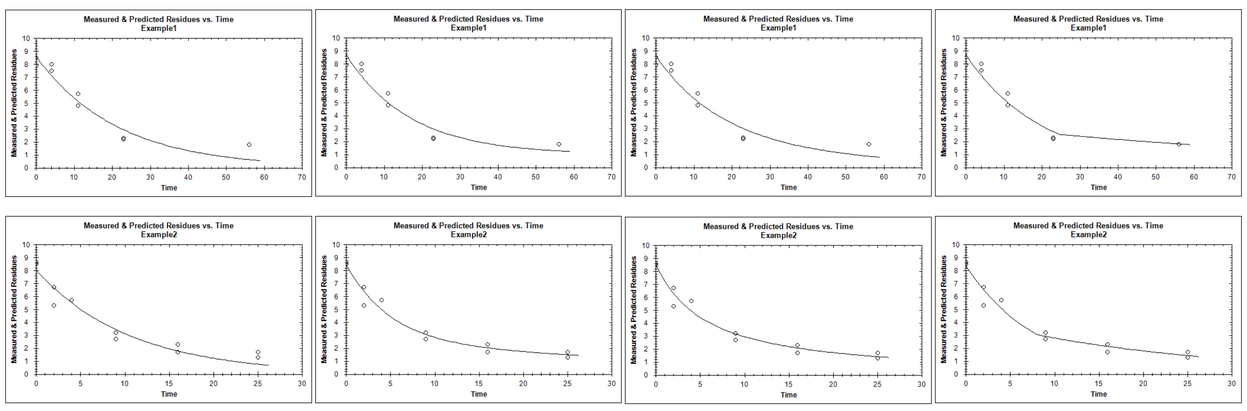
SFO or bi-phasic kinetics?

Degradation of a parent substance in two different soils was assessed in this example extracted from a current Renewal Assessment Report, before the EFSA conclusion has been finalised, which resulted in the applicant and RMS reaching different conclusions on the selection of kinetics from each soil:

SFO DFOP FOMC HS



Parameter	SFO	DFOP	FOMC	HS
Visual Fit	Yes	Yes	Yes	Yes
Residuals	Yes	Yes	Yes	Yes
χ^2	9.11	9.35	9.50	7.66
M0	8.60	8.70	8.64	8.70
k1 (or α)	0.047	0.059	6.06	0.05
k2 (or β)	-	<0.001	120.09	0.011
tb / g	-	0.887	-	24.56
t-test for k1 / k2	Pass	Fail, Fail	-	Pass, Fail
DT50	14.75	13.98	14.50	13.82
DT90	49.01	-	55.49	122.56
Trigger DT50	14.75	13.98		

Parameter	SFO	DFOP	FOMC	HS
Visual Fit	Yes	Yes	Yes	Yes
Residuals	Yes	Yes	Yes	Yes
χ^2	9.86	5.73	5.43	6.26
M0	8.60	8.44	8.51	8.36
k1 (or α)	0.095	0.202	1.148	0.125
k2 (or β)	-	0.023	6.544	0.045
tb / g	-	0.696	-	8.11
t-test for k1 / k2	Pass	Fail, Fail	-	Pass, Pass
DT50	7.32	5.46	5.43	5.52
DT90	24.35	48.39	42.09	36.89
Modelling DT50	7.32			15.4 (k2)

- First soil – applicant rejected SFO, but RMS chose SFO for trigger endpoint
- Second soil – applicant accepted SFO, but RMS chose the slow phase from the HS fit for the modelling endpoint
- Based on the same data, assessment by two different experts (the applicant and the RMS) may result in significantly different DT50 values

Experience with field data

EFSA (2014)[1] guidance on combining DegT50 field values with DegT50 lab values:
Recently published data for 12 active substances (a.s.) with field data for at least the parent were reviewed to check guidance implementation. Of these:

- DegT50 values were combined for 4 a.s.
- DegT50 lab was used for 7 a.s. & DegT50 field was used for 1 a.s.

Reasons for not combining:

- Statistically significant difference between field and lab values (1 a.s.)
- No DegT50 field available from field studies (4 a.s.)
- Stated in published data to be "not relevant/not tested" (3 a.s.)

Origin of DegT50 for PEC modelling	Number of a.s.	Evaluated acc. to EFSA (2014)	Source in AIR process		
			EFSA conclusions	RAR**	SSSD***
Combined	4	4	3	-	1
DegT50 lab	7	0*	2	3	2
DegT50 field	1	1	1	-	-

* see "Reasons for not combining", ** draft Renewal Assessment Report, *** Sanitised Supplementary Summary Dossier

Possible improvements: - Documentation on combining DegT50 values provided in evaluation / summary reports is very scarce.
- Averaging of formation fractions for metabolites (when combining DegT50 values is possible) is not covered by guidance.

EFSA (2016)[2] draft guidance for exposure assessment of soil organisms recommends use of geomean modelling DegT50 values with new exposure tools vs currently using max. non-normalised DisT50 or DegT50 values. Potential impact on PECsoil was assessed with the same 12 substances.

- DegT50 values always shorter than DT50 values used for PECsoil calc.
- Effect of shorter DegT50 likely to be compensated by conservatism implemented in new exposure assessment scheme for soil organisms

Scale factor: DegT50 → DT50	Number of a.s.	Source in AIR process		
		EFSA conclusions	RAR	SSSD
x 1.8-3.6	6	3	1	2
x 4.8-8.7	5	2	2	1
Not relevant, only initial PECsoil evaluated	1	1	-	-

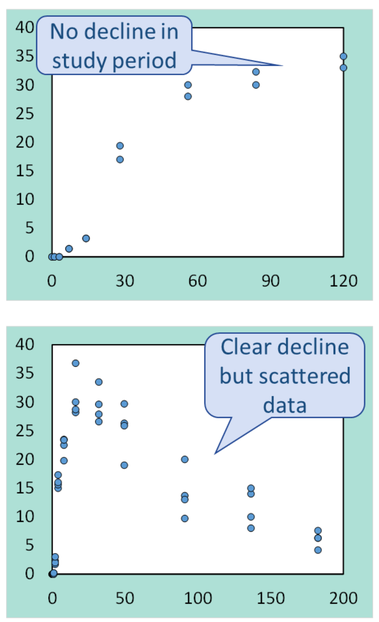
Challenges for metabolites

'Difficult' kinetics:

Complex pathways
No decline at end of study
Small or scattered residues
Bi-phasic metabolites

Non-robust fits:

Relax t-test or chi^2 criteria?
Default DegT50 and formation fraction?
What is a 'reasonable worst-case'?
Use evidence from other soils?



Conclusions

FOCUS degradation kinetics guidance greatly improved harmonisation.

Differences in interpretation exist, with implications for all parts of the environmental risk assessment.

Constantly evolving area due to new regulations, guidances and tools.

Outlook

New Generic FOCUS guidance co-ordinated by UK CRD will provide clarity and aims to reduce user subjectivity in decision making.

Draft proposal until agreed with EU Member States and EFSA.

1 EFSA, 2014. EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662, 37 pp., doi:10.2903/j.efsa.2014.3662
2 EFSA, 2016. Draft EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal.