

Validation status of TKTD models

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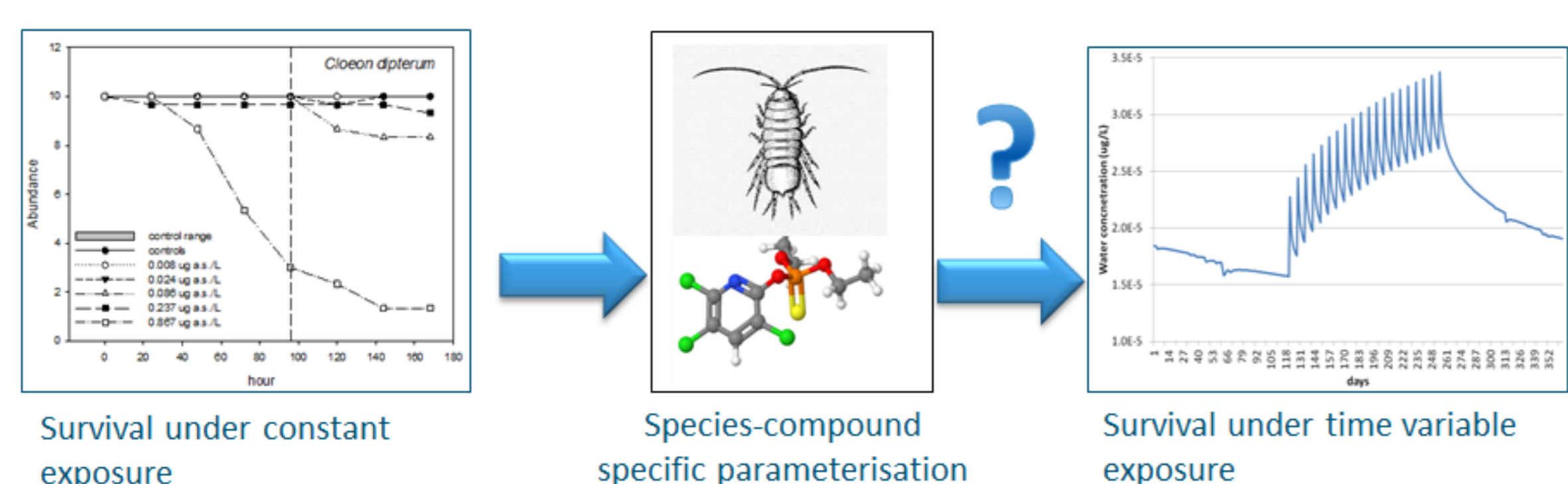
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Background & Objectives

- TK/TD models are able to deliver relevant information for environmental risk assessment of pesticides, especially for the extrapolation from toxicity observed under constant lab conditions to survival under time-variable exposure as expected for realistic application scenarios. TK/TD models from the GUTS framework describe the expected survival for a number of individuals being exposed to chemical concentrations over time [1,2]. For an application in risk assessment, it is required to validate the parameterised models for specific combinations of compounds and species.
- This study presents validation results for TK/TD models for some sets of species and compounds, including the neonicotinoids imidacloprid, thiamethoxam and thiacloprid, the benzimidazole fungicide carbendazim, the pyrethroid insecticide cypermethrin, and the organophosphate insecticide and acetylcholine esterase inhibitors chlorpyrifos, dimethoate and malathion, using models that were parameterised on standard acute data and using observed survival of individuals under time-variable exposure as validation data sets.
- Objective of this work : give an overview of the validation status of GUTS models and to analyse the validation results for patterns of prediction qualities across different compound classes and species.

Methodology

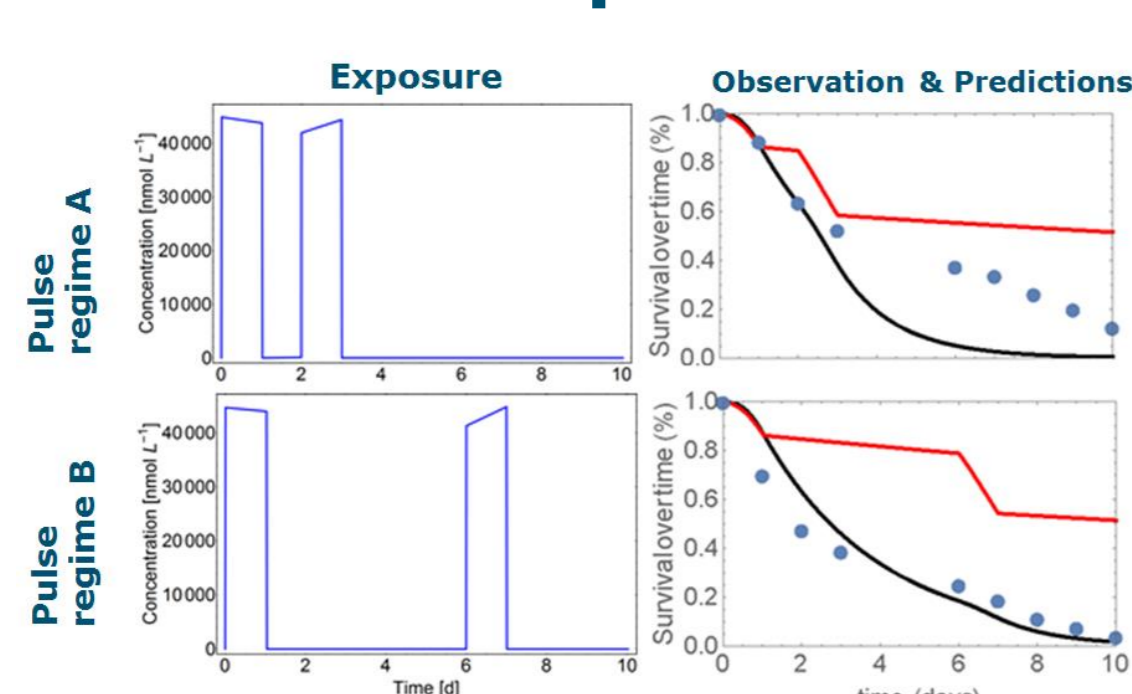
Principle



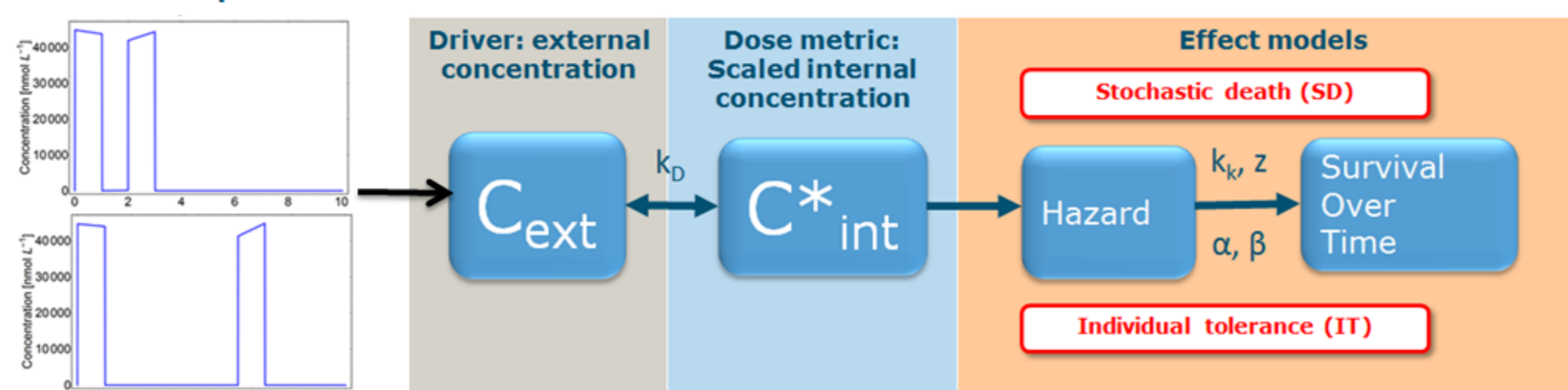
Species, compounds and data sources

Compound	Tested species	Reference
Chlorpyrifos (CPF)	<i>Asellus aquaticus</i> , <i>Gammarus pulex</i> , <i>Chaoborus obscuripes</i> , <i>Plea minutissima</i> , <i>Cloeon dipterum</i> , <i>Daphnia magna</i> , <i>Neocaridina</i>	[4,5,6]
Imidacloprid (IMI)	<i>Asellus aquaticus</i> , <i>Caenis horaria</i> , <i>Chaoborus obscuripes</i> , <i>Cloeon dipterum</i> , <i>Plea minutissima</i>	[3] + unpublished data
Thiacloprid (TC)	<i>Cloeon dipterum</i>	
Thiamethoxam (TM)	<i>Cloeon dipterum</i>	
Carbendazim (CBZ)		
Cypermethrin (CYP)	<i>Gammarus pulex</i>	[2]
Dimethoate (DIM)		
Malathion (MAL)		

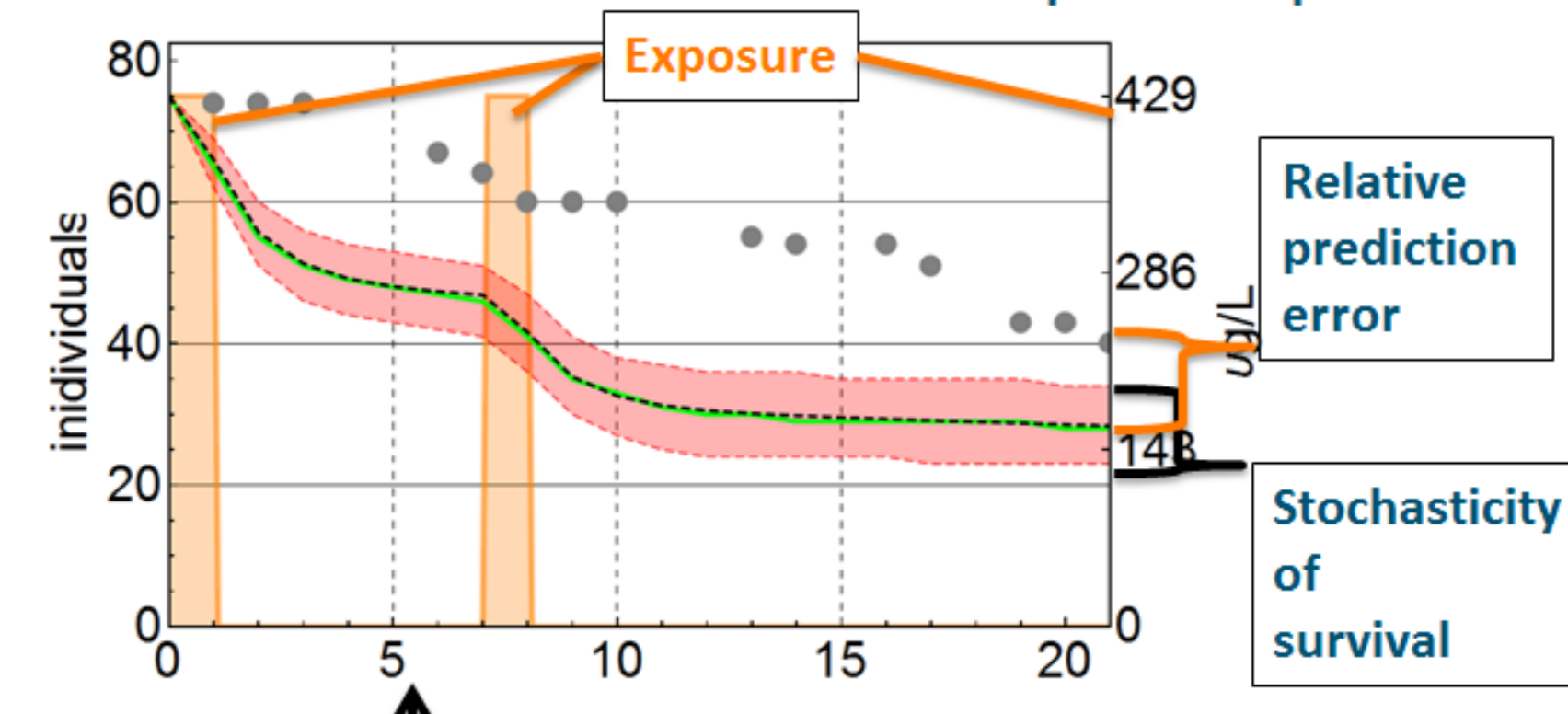
Validation experiments



Exposure time series from validation experiments

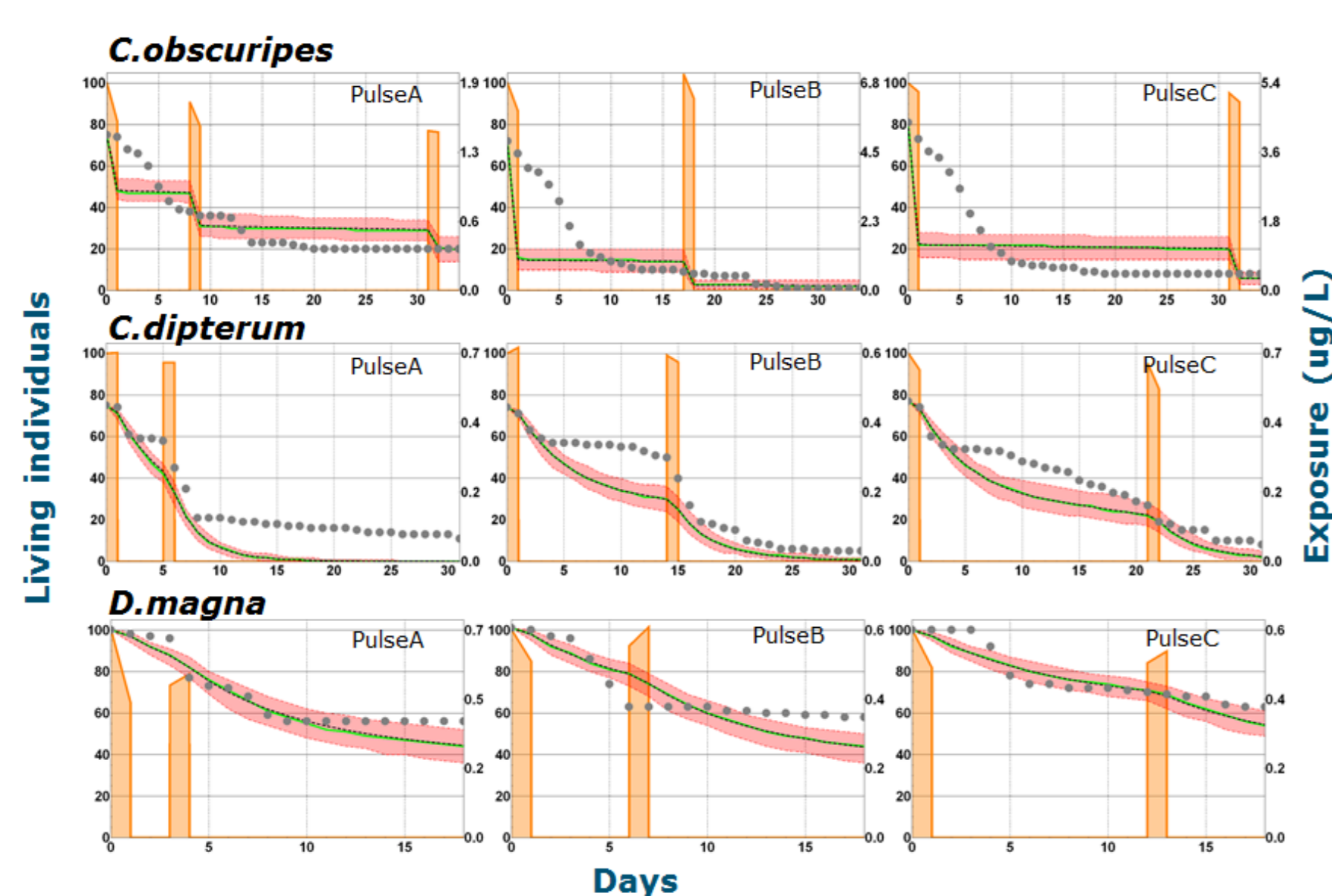


Prediction of survival over time under specified exposure

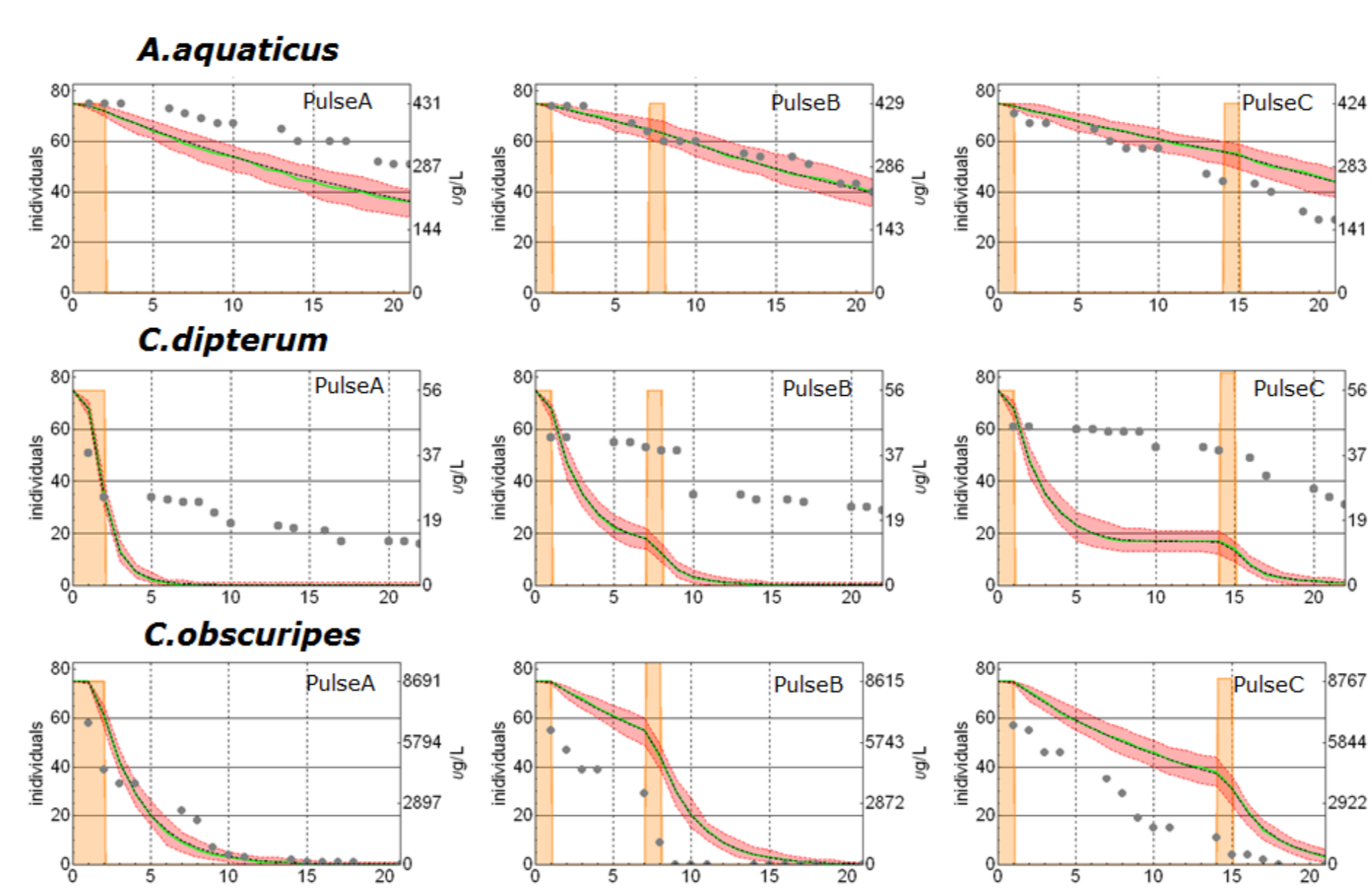


Results and Discussion

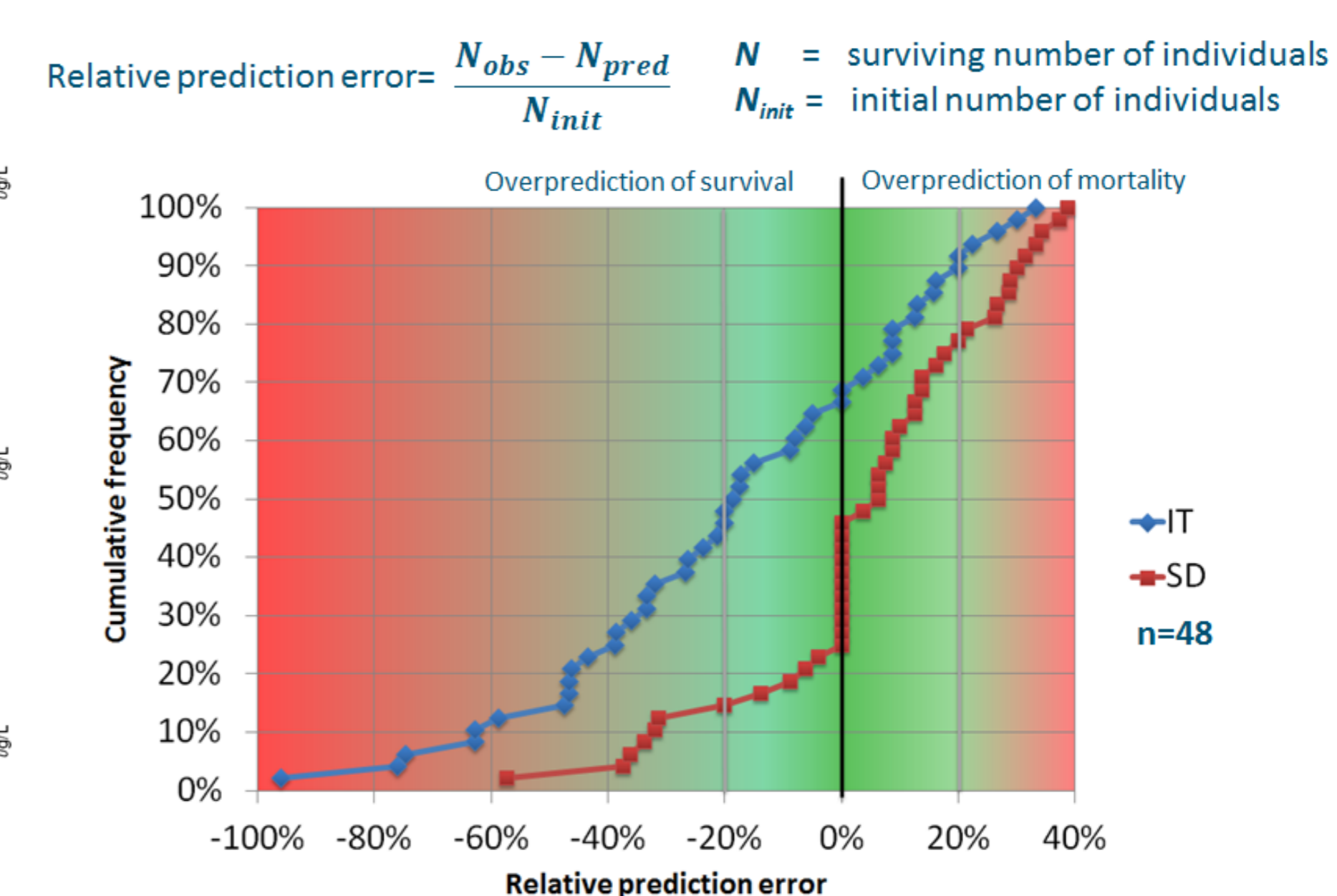
Chlorpyrifos and some species



Imidacloprid and some species



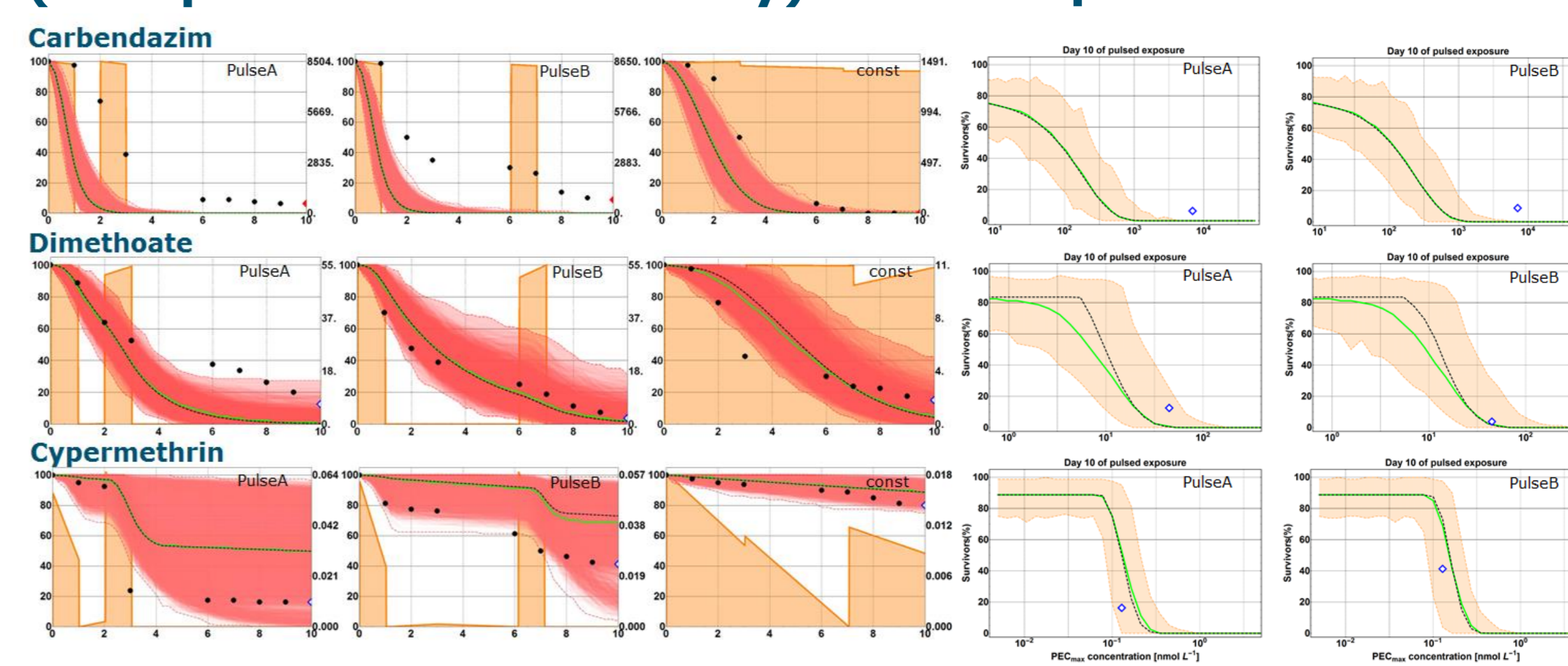
Validation summary



Conclusions and Outlook

- Validation** - Predictions of survival under time-variable exposure do not always match the observed time course, but the majority of SIC-SD predictions (n=31/48) of the mortality at the end of the exposure match observations within $\pm 20\%$
- Impact assessment** - How are toxicity thresholds of experiments and TK/TD model results related? TK/TD toxicity thresholds can be compared with all effect assessment tiers (and particularly the surrogate reference tier)
- Standardisation** - TK/TD modelling as presented can be standardized based on standard toxicity data
- Usefulness** - TK/TD modelling evaluates the complete exposure information - for complex exposure patterns more useful than PEC_{max} or TWA
- Uncertainty** - Parameter uncertainty and exposure uncertainty can be incorporated into model predictions [2]; Margins of safety can be calculated, i.e. how far is an exposure from causing an effect [7]
- Screening** - large numbers of scenarios can be screened based on TK/TD models, e.g. for the whole (national) area of use of a compound

G. pulex and some compounds (incl. parameter uncertainty)



G. pulex - the dose - response view

GUTS is a dose-response model, just better...

References

- [1] Jager T, Albert C, Preuss TG, Ashauer R. 2011. ES&T 45:2529-2540. [2] Ashauer, R. et al. Modelling survival: exposure pattern, species sensitivity and uncertainty. Scientific Reports 6, 29178, (2016). [3] Van den Brink PJ, Van Smeden JM, Bekele RS, Dierick W, De Gelder DM, Noteboom M, Roessink. 2015. ET&C. DOI: 10.1002/etc.3152 [4] Ashauer R, Boxall AB, Brown CD. 2007. ES&T 41:1480-1486 [5] Zafar, MI, PhD thesis, Wageningen University, Wageningen, NL (2012) ISBN 978-94-6173-371-9 [6] Rubach MN, PhD thesis, Wageningen University, Wageningen, NL (2012) ISBN 978-90-8585-767-9 [7] Ashauer et al. (2013) ET&C 32(4):954-965.

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