Bridging the gap across species by the means of TK-TD modelling

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Introduction

- Aquatic effect assessment uses results from laboratory experiments
- Test organisms are kept under constant environmental conditions which might differ across species (e.g. optimal temperature)
- Results are used to statistically derive community level endpoints (e.g. HC5 from species sensitivity distributions (SSDs))
- LC_{50}s have been reported to depend on ambient temperature [1] → problems when comparing species sensitivities
- Changes in physiological rates at different temperature regimes can be described by the Arrhenius function [2]
- Extrapolation of toxicity across species can be done using the connection of the threshold z and the volume-specific somatic maintenance rate pM which resembles the metabolic rate

Material & Methods

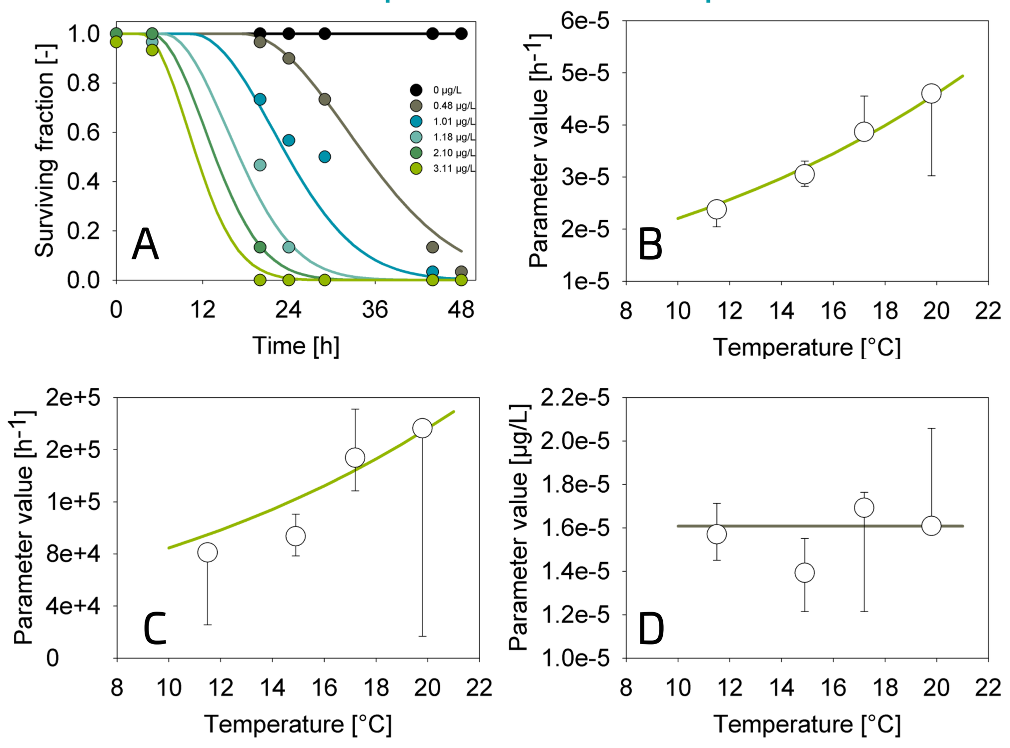
- 10 aquatic species
- Temperature range: 12-25°C
- Chlorpyrifos
- GUTS [3] with SIC and SD
- SSD generator [4]
- DEB IBM *Daphnia magna*

Conclusions

- Temperature correction of GUTS parameters allows for a direct comparison of toxicity across species.
- Temperature correction altered the rank order of species within the SSD
- The correction is particularly needed in low temperatures, otherwise risk might be underestimated
- Temperature correction has the potential to reduce uncertainty in the derivation of endpoints such as the HC_5
- Scaling of the threshold parameter with the metabolic rate pM allows for a cross species extrapolation of toxicity
- The inter-correlation of GUTS parameters would allow the prediction of effect for untested species and exposure scenarios
- Individual based models facilitate the extrapolation of higher level effects from individual level toxicity testing.
- Prediction of population level effects for untested species is deemed possible if the uncertainty in parameter estimation is accounted for in the cross species-correlation.
- The applicability of the approach is demonstrated for the example of Chlorpyrifos, its generality needs however been tested in future trials.

Temperature dependency

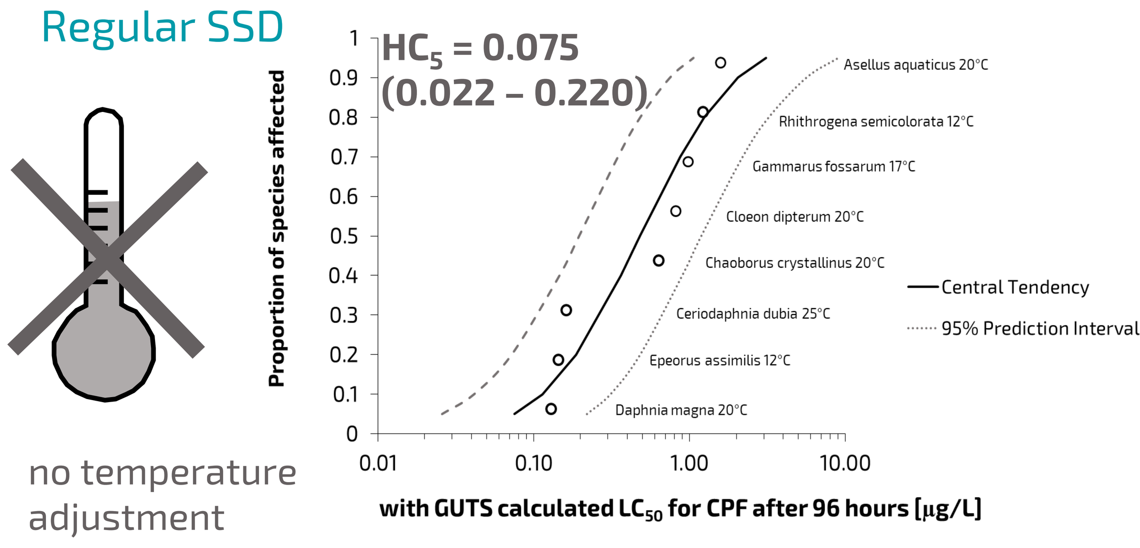
GUTS model predictions and parameters



A GUTS model fit for 48 hours toxicity test with *D. magna* and Chlorpyrifos at 17 °C.
B dominant rate constant k_e
C slope parameter k_k
D effect threshold z

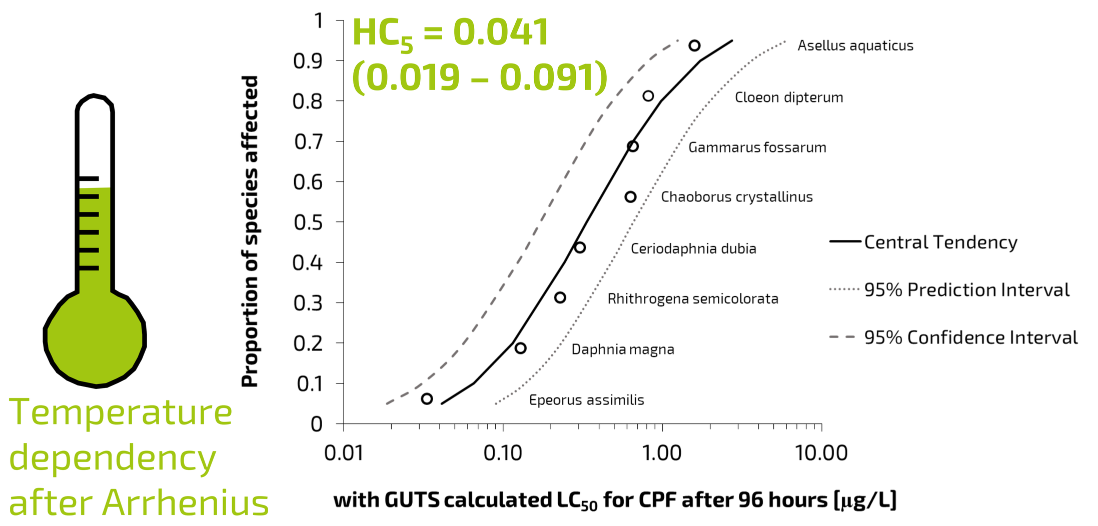
O Parameter values
— Arrhenius model prediction based on 20°C parameter
— Constant temperature prediction based on 20°C parameter

Regular SSD



SSD of 8 aquatic invertebrates regarding Chlorpyrifos based on LC_{50} 96h values calculated with GUTS. Measured concentration in microgram per litre (log-scale) and affected fraction. Temperature range: 12—25°C

Temperature corrected SSD

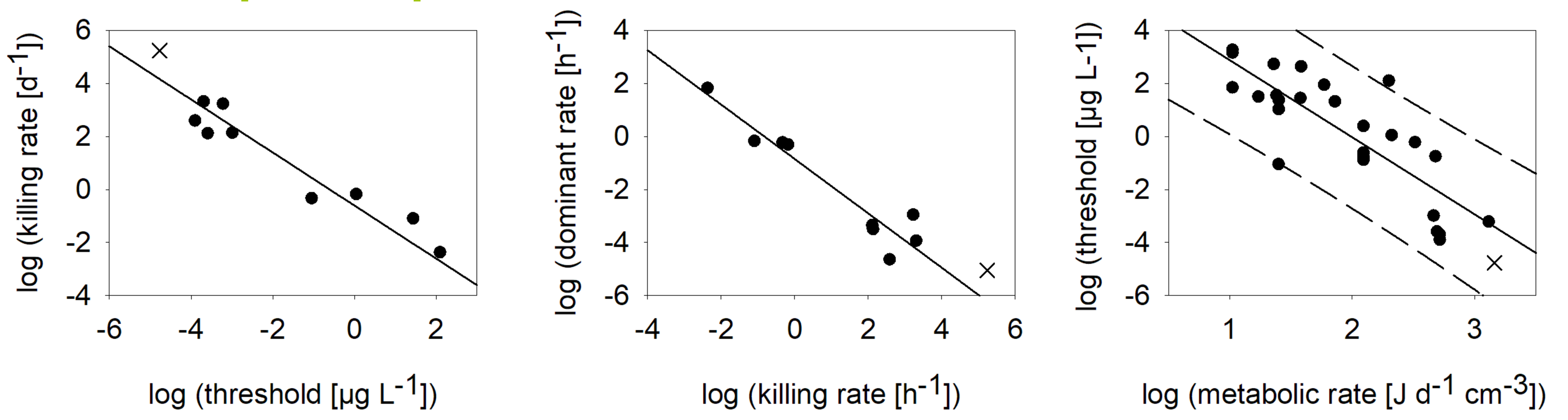


SSD of 8 aquatic invertebrates regarding Chlorpyrifos based on LC_{50} 96h values calculated with GUTS. Measured concentration in microgram per litre (log-scale) and affected fraction. Temperature range: 12—25°C

- The GUTS parameters k_e and k_k show temperature dependency which can be predicted by Arrhenius function for *Daphnia magna*
- GUTS parameter *z* is independent of temperature
- EC_{50} values of *Daphnia magna* show temperature dependency

- Temperature adjustment of the GUTS parameters k_e and k_k resulted in different LC_{50}s (the higher the temperature the more sensitive is the organism to a toxicant) which then induced a shift in the SSD
- HC_5 from SSD is affected, noticeable in a lower value and smaller range of the prediction intervals

Cross species parameter correlations



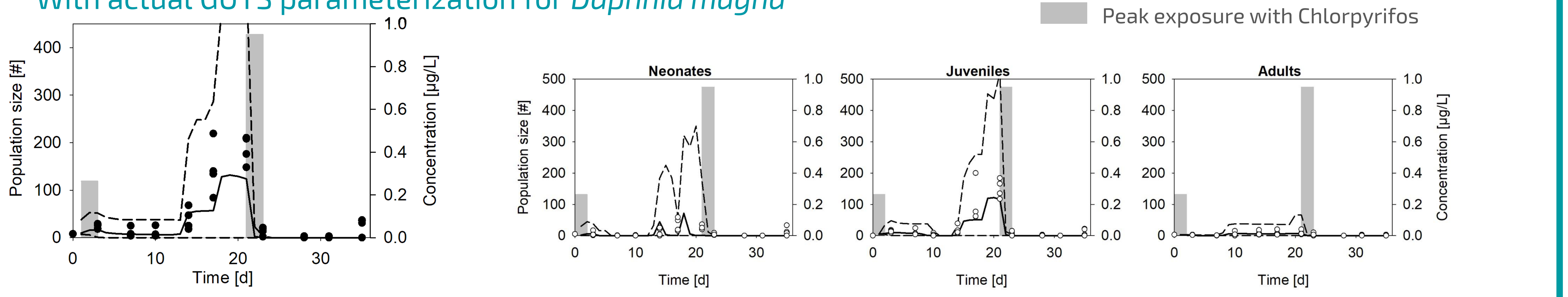
● Parameter values used in regressions [5]
× *D. magna* parameter values

- GUTS parameter correlations for chlorpyrifos
- The correlation of the threshold z with pM [6] allows for calculation of parameters from untested species

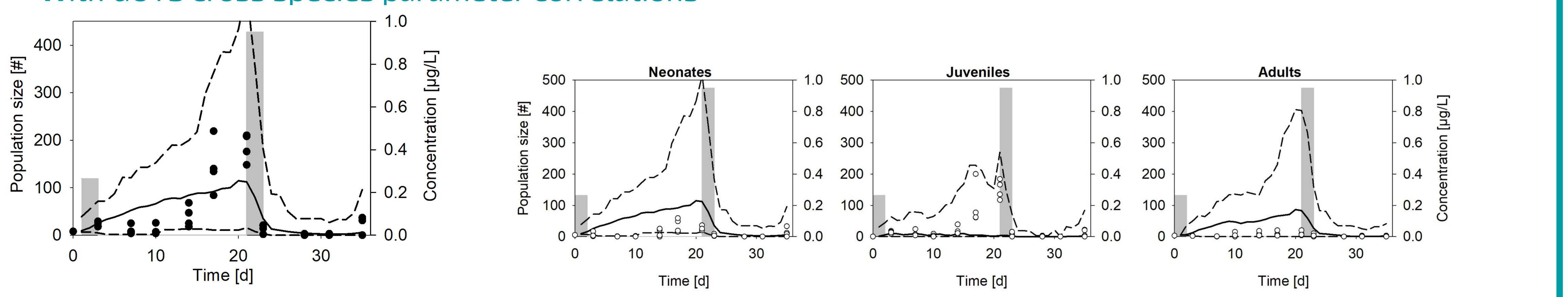
Population level extrapolations with DEB IBM *Daphnia magna*

● data
IBM predictions: mean, minimum, maximum
Peak exposure with Chlorpyrifos

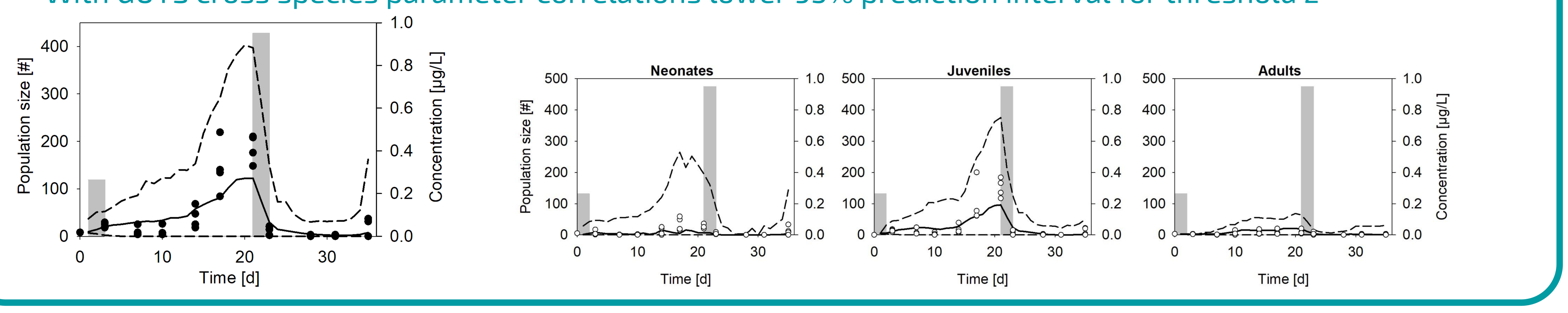
With actual GUTS parameterization for *Daphnia magna*



With GUTS cross species parameter correlations



With GUTS cross species parameter correlations lower 95% prediction interval for threshold z



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