Predictive modelling of metal mixture toxicity to *Daphnia magna* populations

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1. Introduction

Current practice of environmental risk assessment lacks ecological realism, because it depends mostly on toxicity of single substances to individual organisms.[1] It is desirable to develop mechanistic, predictive models accounting for mixture toxicity on higher levels of organization. The goal of this research was to identify the capacity of a Dynamic Energy Budget Individual-Based Model (DEB-IBM) to predict toxicity of Cu-Ni-Zn mixtures to *Daphnia magna* populations, if only calibrated with single metal data, while making use of available model parameters for *D. magna*. We conducted a population experiment with *D. magna* exposed to Cu-Ni-Zn mixtures and the single metals. Correction factors were determined for selected DEB-IBM parameters. Predictions of mixture toxicity were generated with the DEB-IBM, as well as the reference models Independent Action (IA) and Concentration Addition (CA). The predictive performance of the DEB-IBM and possible improvements on the calibration procedure are discussed.

2. Materials and methods

2.1. Population experiment

D. magna populations were exposed for 6 weeks in 500 mL of modified COMBO medium (4 mg natural DOC/L, 15 mg Ca/L, 11 mg Mg/L, 0.175 mg B/L, pH adjusted to 7.5 without buffer). Populations were fed daily with a mix of *Raphidocelis subcapitata* (8.3×10^7 cells/L) and *Chlamydomonas reinhardtii* (3.5×10^7 cells/L). 25% of media were renewed and population densities were determined twice a week. Metal concentrations were arranged in a single ray design (5 concentrations, fixed ratio of 1:1:3 Cu:Ni:Zn). Analysis was done based on mean measured dissolved concentrations (ICP-OES, samples passed through 0.45 µm filter).

2.2. Statistics and modelling

Log-logistic dose-response models were fitted to final population density under single-metal exposure, to generate Independent Action (IA)- and Concentration Addition (CA)-predicted responses.[2] To calibrate the DEB-IBM [3] with population data, parameter combinations were sampled from separate prior distributions. By extracting a fraction of parameter values with the best fit, posterior distributions for the parameter estimates were generated. This was done with 1. maximum surface area-specific assimilation rate and half-saturation constant of the functional response, 2. parameters for lethal effects of Cu and Zn, 3. dose-response parameters for sub-lethal effects of Ni on growth. As default values, previously determined parameter values for *D. magna* were adopted from Pereira et *al.* [4] and in-house data (Karel Vlaeminck, unpublished). Metals with different physiological modes of action (PMoA) were implemented independently. For metals with identical PMoA, we assumed no interactions between metals [5], corresponding to IA on a sub-physiological level. Refinement of the calibration approach is ongoing.

3. Results and discussion

Figure 1 shows observed responses of population densities after 6 weeks, with predictions of the DEB-IBM and reference models. By applying simple corrections to toxicity parameters, qualitatively adequate fits could be achieved for Cu and Zn, but not for Ni. This can point at different issues in calibration, such as inappropriate choice of PMoA or lack of direct sub-lethal effects of Ni. Predictions of mixture toxicity were less conservative than IA and CA, especially for intermediate concentrations (Figure 2). Accuracy of CA and IA were concentration-dependent. In contrast to descriptive models, DEB-IBMs have the capacity to capture such trends. Mixture toxicity at the population level is not only the result of combined effect of toxicants, but potentially also of interaction between organisms, such as competition for food, [6] which can be accounted for in IBMs. Response to mixtures at the individual level emerges from physiological processes (assuming IA or CA on the sub-physiological level), and does thus not necessarily match either IA- or CA-predicted responses on the individual or population level.[5]

4. Conclusions

While descriptive models of mixture toxicity (CA and IA) are limited in their predictive power, DEB-IBMs can potentially cover a wider range of scenarios, giving the opportunity to test the predictiveness of the DEB-IBM in comparison to CA and IA. In our dataset, both reference models were conservative, but neither provided satisfying predictions across the entire range of tested concentrations. We conclude that this approach is more likely to result in models that predict mixture toxicity across levels of organization and exposure scenarios than purely descriptive models. A calibration with simple correction factors of selected parameters has not shown to be sufficient. Calibration of all toxicity parameters, as well as the appropriate choice of PMoA, have to be explored to reach more satisfying blind predictions.

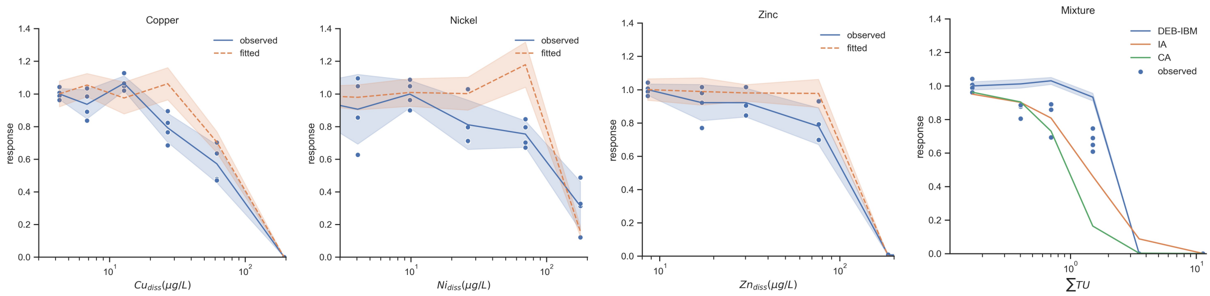

Figure 1 Observed and predicted response of population density after 6 weeks for single metals and the mixture. Lines indicate averages, ribbons indicate standard deviation. After preliminary calibration, the DEB-IBM was not conservative at low and intermediate concentrations.

References

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