

SITE-SPECIFIC RISK ASSESSMENT OF LEAD IN SURFACE WATERS WITH BLM-TOOL PNECpro V6.

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Introduction

PNEC.pro is a user-friendly tool for professionals dealing with the assessment of surface water quality (Vink et al., 2013). It calculates local, water-type specific no observed effect concentrations (NOECs) for various metals, based on the full biotic ligand model (BLM) simplifications of Verschoor et al. (2012). With the upcoming update, the bioavailability calculations for lead will be implemented in the tool. Lead (Pb) is a priority substance of the European Water Framework Directive (European Union, 2013). With the revision of 2013, it is required that the environmental quality standards for lead in surface waters are based on bioavailable concentrations. Full-BLMs for lead are available for various organisms. However, the BLM procedure is complex, and detailed toxicity databases are required. Moreover, the procedure includes sophisticated chemical speciation calculations and many input parameters are required. Therefore, a large amount of full BLM calculations were used to derive simplified functions that perform with good reproducibility, using only a limited number of easily measured water characteristics.

Methods

The well-screened chronic toxicity dataset from the European Union Voluntary Risk Assessment Report for Pb and Pb compounds (EU VRAR, 2008) was used. It contains 159 chronic lead toxicity test results (NOEC/EC10) for 25 aquatic species. For full BLM modelling, we used the models for algal species (*Pseudokirchneriella subcapitata*; De Schamphelaere et al., 2014), daphnid (*Ceriodaphnia dubia*; Nys et al., 2014) and fish (Fathead minnow, *Pimephales promelas*; Van Sprang et al., 2015). Chemical speciation calculations were performed with Visual Minteq3.1, and complexation with dissolved organic matter (DOM) was calculated with the NICA-Donnan formulation to acquire free Pb²⁺ concentrations. The BLM model parameters (log KHBL; log KCaBL; SpH) were used to calculate binding to the respective biotic ligands.

A large hypothetical water quality database was created to derive simplified equations from the full BLM results. The database was created using R version 3.2.2. This database contained all possible combinations of relevant water characteristics that influence site-specific speciation of lead. Limits of pH and Ca were set on the validated range of the underlying BLM models, and evenly distributed in the database. Full BLM calculations, containing nonlinear equations, were simplified by transforming them into linear equations for HC5. Multivariate analyses were performed to select the most relevant water characteristics. Whether the addition of a parameter significantly improved the model was determined by the Akaike Information Criterion. The general formula for these simplified transfer functions is:

$$HC5 = a + (b \times par_1) + (c \times par_2) + (d \times par_3) + \dots + (I \times par_n)$$

The acquired transfer functions were evaluated by applying them to seven European "ecoregions". These are selected databases that were used in the European Risk Assessment Report for model validation purposes.

Results

Results are shown in Table 1 and Figure 1.

Table 1. HC5 values ($\mu\text{g/L}$) calculated by full BLM modelling, and estimated by some selected 1-, 2-, and 3-parameter transfer functions for seven European ecoregions.

| Model | River Teme (UK) | River Otter (UK) | River Rhine (NL) | River Ebro (ES) | Ditch (NL) | Acidic lake (SE) | Lake Monate (IT) |
|-----------------------------|-----------------|------------------|------------------|-----------------|-------------|------------------|------------------|
| Full-BLM^a | 17.6 | 8.9 | 6.4 | 6.5 | 31.9 | 11.4 | 8.3 |
| <i>functions</i> | | | | | | | |
| DOC + Ca + Na | 19.0 | 7.6 | 4.8 | 6.0 | 28.7 | 12.8 | 9.0 |
| DOC + pH + Ca | 19.5 | 7.7 | 5.5 | 7.4 | 29.0 | 11.9 | 8.1 |
| DOC + pH + Mg | 19.6 | 7.2 | 6.5 | 7.7 | 28.5 | 10.6 | 6.4 |
| DOC + Ca | 19.7 | 8.1 | 5.7 | 7.7 | 28.9 | 12.1 | 8.6 |
| DOC + Mg | 20.2 | 8.1 | 7.2 | 8.5 | 28.2 | 10.6 | 7.2 |
| DOC + pH | 19.4 | 6.9 | 6.3 | 8.0 | 30.1 | 10.4 | 5.7 |
| DOC + Na | 19.9 | 8.2 | 7.0 | 9.5 | 29.4 | 9.7 | 6.6 |
| DOC | 19.8 | 8.0 | 7.0 | 9.2 | 29.6 | 9.5 | 6.3 |

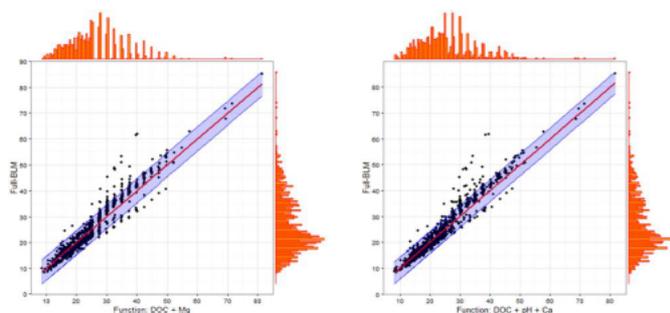


Figure 1. Statistical comparison between full BLM computations and estimations by simplified functions. Histograms show distribution of data points; P95 confidence interval (bleu area); and 1:1 fit (red line).

Conclusions

Full BLM computations of Pb, performed with detailed toxicity databases and complex chemical speciation routines, could be closely simulated by 1-, 2-, and 3-parameter transfer functions. These functions provide robust tools for higher-tiered risk assessment in surface waters of various compositions.

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