Inclusion of metabolites in the assessment of bioaccumulation and biological activity

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Introduction

Bioaccumulation is often used as an indicator of ecotoxicological risk. Within the concept of ecotoxicological risk profiles [1, 2, 3], this indicator is complemented by the risk indicators release R, spatiotemporal range S, biological activity B and uncertainty U.

Such a use of five indicators covers the whole pathway relevant for the decisions on ecotoxicological risks, starting from information about the entry of the substance into the environment up to reflexive information about the quality of the evaluation (Figure 1).

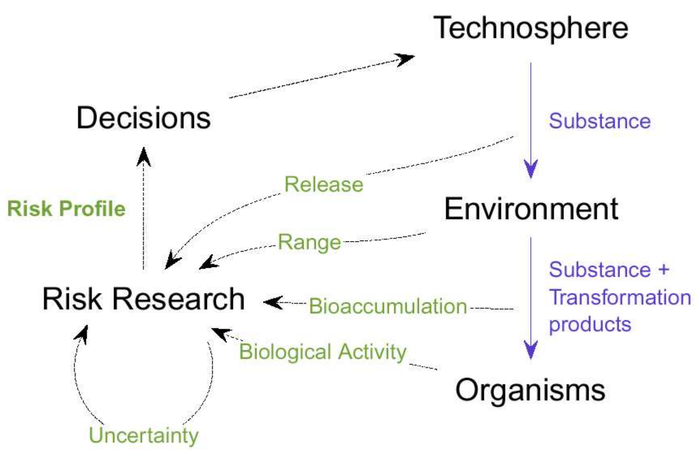

Figure 1: The information cycle of risk management along the pathway of environmental chemicals

While the release indicator R only deals with the estimated global release rate I of the *original* substance,

$$\mathsf{R} \propto \log_{10} I \tag{1}$$

the spatiotemporal range S includes *transformation products*. It can be perceived as the total amount of the substance and its relevant transformation products in the environment in steady state n_{env}, divided by its release rate, or, in other words, the joint residence time t_{joint} of the substance and its relevant transformation products within a model of the global environment (cp [4]).

$$\mathsf{S} \propto \log_{10} \frac{n_{\mathrm{env}}}{I} = \log_{10} t_{\mathrm{joint}} \tag{2}$$

Strictly following this train of thought, the bioaccumulation indicator B is defined as the quotient of the total amount of the substance including relevant transformation products present in organisms in steady state n_{bio}, divided by the total amount in the environment n_{env} as defined above.

$$\mathsf{B} \propto \log_{10} \frac{n_{\mathrm{bio}}}{n_{\mathrm{env}}} \tag{3}$$

Perceived in this manner, bioaccumulation as a risk indicator strongly depends on transformation reactions of the original substance as well as on the partitioning, uptake and clearance of transformation products. Only by virtue of this definition, highly bioaccumulating transformation products will directly contribute to the risk caused by the release of the original substance and substances with persistent metabolites and a correspondingly high spatiotemporal range will be judged by a ”fair” metric of their bioaccumulation.

Taking it one step further, the indicator biological activity A should indicate the biological effects resulting from these substances present within the organisms, i.e. resulting from their total internal exposure.

Methodological approach

In this contribution, mathematical formulae for the estimation of thusly defined indicators are presented. Strategies for assessing biological activity from simultaneous measurements of biological effects and internal exposure are given special attention.

Relevance of transformation products

The question which of the known or suspected transformation products should be included in an assessment of joint persistence [4], secondary persistence [5] or spatiotemporal range [2], has not been answered in a general manner, so it is up to the risk researcher to judge which of them are regarded irrelevant for the risk assessment.

Modelling joint bioaccumulation

For the evaluation of the spatiotemporal range of the substance according to the definition given above (eqation 3), a fate model of the form

$$\dot{\mathbf{n}} = f(\mathbf{n}) + \mathbf{S} \tag{4}$$

can be defined, where $\mathbf{n}$ is a vector of the number of moles of each substance i in each model compartment j, therefore containing i times j elements. $f(\mathbf{n})$ contains descriptions of the change in number of moles in each compartment in dependence of the amount of every substance in every compartment. $\mathbf{S}$ is the source term, which has to be constant over time for a steady state solution.

Recently, not only fish biomass but also vegetation is being included in multimedia fate models, so the number of moles terms of equation 3 could be directly derived from steady state solutions of such models.

However, it is often unrealistic to assume that environmental loads will reach steady state concentrations within any period of interest for the decision-maker. Therefore, it is suggested here to use a numerical solution of the model defined according to equation 4 to estimate $\mathbf{n}(t)$ and to estimate the joint bioaccumulation according to equation 3 from $\mathbf{n}(t = 100\mathrm{y})$, assuming a realistic $\mathbf{n}(0)$ and a realistic source term $\mathbf{S}$ according to present knowledge.

This procedure for the evaluation of the risk indicator B is roughly equivalent to weighting the bioconcentration factors for the different compartments with the fractions of the substance present in them, but in addition allows for the inclusion of transformation products in favor of estimating a joint bioaccumulation.

Joint biological activity

Recently, increased attention has been focused on internal effect concentrations. Reasons for this are lower variabilities in internal effect concentrations as compared to external effect concentrations and the possiblity to combine biomimetic extraction for the estimation of total body residues (TBR) of complex contaminant mixtures with internal effect concentrations for the risk assessment of complex mixtures as e.g. effluents (compare e.g. [6]).

In the context of ecotoxicological risk profiles, internal effect concentrations have been chosen as measures for biological activity since they are much more independent of bioaccumulation measures than external effect concentrations.

The problem for a joint assessment of the biological activity of a substance together with its transformation products is that information about toxic effects not only for different biological species (living in different ecological contexts) has to be integrated, but also information for different chemical substances.

One conceptually possible solution of this dilemma is to calculate a weighted average of all internal effect concentrations with weights according to the fraction of the respective substance of the overall mass and according to the relevance of the species with regard to the predicted/known distribution pattern across the environmental media. This approach would be an extension of the one used in the original definition of the ecotoxicological risk profiles [2, 3].

Another approach newly presented here is to build an average of the critical biomasses m^{crit} which are defined here as the biomass needed to dilute one mole of a chemical to a degree that no adverse chronic effect can be observed.

$$\mathsf{A} \propto \sum_{k,j} f_{k,j} \cdot m_{k,j}^{\mathrm{crit}} \tag{5}$$

In the above definition, k is an index over all biomass compartments of the model, j is the indicator over the substances (original plus transformation products), $f_{k,j}$ is the fraction of substance j in biomass compartment k of the total accumulated number of moles n_{bio} and $m_{k,j}^{\mathrm{crit}}$ is the critical biomass volume of substance j in biomass type k as defined above. $V_{k,j}^{\mathrm{crit}}$ values are specific for each type of biomass which is considered by the fate model.

This definition is inspired by the life cycle assessment (LCA) method of critical volumes, where the effects of emissions to the environment are summed up using their critical volumes as weights, calculated from limit values for their concentrations in different environmental media.

It also draws some validity on the assumption that the bioaccumulated mass of substances with equal mode of action can just be added up regardless of their exact identity, as put forward in [6].

Concluding remarks

The main point of generating ecotoxicological risk profiles rather than estimating risk ratios is the need for a method which can cope with partial and uncertain information without producing misleading results. The method is meant to inform decision-makers during the development of chemical products and processes as well as for regulators concerned with the global environmental risk of the release of chemicals.

References

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