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RESEARCH AND EDUCATION HIGHLIGHTS

The ChimERA project: coupling mechanistic exposure and effect models into an integrated platform for ecological risk assessment

F. De Laender · Paul J. van den Brink · Colin R. Janssen · Antonio Di Guardo

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Abstract Current techniques for the ecological risk assessment of chemical substances are often criticised for their lack of environmental realism, ecological relevance and methodological accuracy. ChimERA is a 3-year project (2013–2016), funded by Cefic's Long Range Initiative (LRI) that aims to address some of these concerns by developing and testing mechanistic fate and effect models, and coupling of these models into one integrated platform for risk assessment. This paper discusses the backdrop against which this project was initiated and lists its objectives and planned methodology.

Responsible editor: Philippe Garrigues

F. De Laender (✉) · C. R. Janssen
GhenToxLab, Ghent University, 9000 Ghent, Belgium
e-mail: frederik.delaender@unamur.be

C. R. Janssen
e-mail: colin.janssen@ugent.be

F. De Laender
Research Unit in Environmental and Evolutionary Biology, University of Namur, 5000 Namur, Belgium

P. J. van den Brink
Alterra, Wageningen University and Research Centre, P.O. box 47, 6700 AA Wageningen, The Netherlands
e-mail: paul.vandenbrink@wur.nl

P. J. van den Brink
Department of Aquatic Ecology and Water Quality Management, Wageningen University, 6700 AA Wageningen, The Netherlands

A. Di Guardo
Department of Science and High Technology, University of Insubria, Via Valleggio 11, 22100 Como, Italy
e-mail: antonio.diguardo@uninsubria.it

Background and motivation

The goal of prospective ecological risk assessment of chemicals (ERA) is to quantify the risk that a concentration of a given chemical would impair on the structure and function of natural ecosystems. Typically, environmental exposure and the expected ecological effects are assessed separately, following procedures laid down in guidance documents (EFSA Panel on Plant Protection Products and their Residues 2013; European Chemicals Agency 2011, 2013; European Medicines Agency 2004). For the last 25 years, the environmental realism, the ecological relevance, and the methodological accuracy of these procedures have been questioned (Cairns 1988; Forbes and Calow 2002; Van Straalen 2003; Van den Brink 2008; De Laender et al. 2008a; Van den Brink et al. 2013; Di Guardo and Hermens 2013). Bearing in mind the ecological and environmental complexity inherent to natural ecosystems, risk assessors increasingly realise that ecological risk cannot be adequately assessed using procedures that disregard most, if not all, of this complexity. In general, these procedures compare single point estimates of exposure (e.g. the predicted exposure concentration or PEC) with ecosystem-level thresholds inferred from toxicity data for individual-level endpoints (e.g. the predicted no effect concentration or PNEC). In a recent opinion paper from the Scientific Committee on Health and Environmental Risks (SCHER), the Scientific Committee on Emerging and Newly Identified Health Risks (SCENIHR), and the Scientific Committee on Consumer Safety (SCCS) of the European Union (SCHER et al. 2013), the challenges related to improving the current ERA practices are discussed in detail. These challenges can be divided into four categories. A first challenge is to more explicitly acknowledge variability in chemical exposure assessment. Indeed, exposure to chemicals is not constant in time and is not homogeneously distributed in space. Different regions may exhibit site-

specific bioavailability-determining physical and chemical characteristics, but also within one region, patterns of chemical emission as well as local variability of environmental conditions may create a spatial and temporal exposure mosaic (Gasic et al. 2009; Morselli et al. 2011). A second challenge relates to the presence of multiple stressors in real ecosystems, as opposed to the presence of single chemicals in the toxicity tests on which prospective ERAs are generally based. The performance of individuals is therefore not solely determined by the presence of individual chemicals but by multiple stressors, including (mixtures of) chemicals (Verbruggen and Van den Brink 2010), possibly targeting different trophic levels (Van den Brink et al. 2009), and other stress factors such as, for example, changes in temperature (Heugens et al. 2001). A third scientific challenge for ERA includes the incorporation of recovery-inducing processes. Recovery may occur at the individual, population, and community level upon removal and/or diminution of the stressor. At the individual level, recovery rates will predominantly depend on the toxicokinetics and toxicodynamics of the chemical (Ashauer et al. 2011). At the population level, the species' life history characteristics and dispersal rates govern recovery rates (Caquet et al. 2007; Galic et al. 2012). At the ecosystem level, recovery of ecosystem functions will be promoted when species within functional groups have different sensitivities towards the chemical (De Laender et al. 2011). A last challenge for ERA deals with closing the gap between individual-level assessment endpoints many ERA procedures are based on and the protection goals listed in regulatory documents (Hommen et al. 2010). For example, individual-level effects on invertebrates are initiators of effects at higher levels of biological organisation, i.e. populations, communities and ecosystems. This propagation of individual-level effects may cause tolerant species or ecosystem functions to be affected due to ecological interactions in the community (Fleeger et al. 2003; De Laender et al. 2010), but likewise functional redundancy among species may compensate species loss and sustain functions in stressed ecosystems (De Laender et al. 2011).

Experimentally examining the effects of multiple stressors at higher levels of biological organisation from multiple exposure scenarios in various geographical areas is an informative exercise for a selection of case studies but cannot be considered as a standard approach for ERA. Instead, when based on first principles and tested against multiple patterns observed in reality, modelling can play a key role in meeting the challenges listed above. Indeed, models can be developed using a limited set of environmental and ecological contexts, after which extrapolation to many different alternative scenarios is possible.

The interest in modelling in the ecotoxicological community increased tremendously over the last decade. Mechanistic modelling of environmental fate and exposure of chemicals has already been accepted as a standard tool for more than 10 years, but now there is increasing awareness that corresponding progress in effect modelling is needed, including the expected effects on individuals (Jager et al. 2011), populations (Forbes et al. 2009; Grimm et al. 2009; Galic et al. 2012), ecosystems containing functional groups in a food-web context (Traas et al. 2004; De Laender et al. 2008b, 2011) and, more recently, on the biodiversity of aquatic plankton communities (De Laender et al. 2013). The EU-funded project CREAM (http:/cream-itn.eu; Grimm et al. 2009) propelled this evolution and a large number of individual- and population-level effect models are now available, some of which are actively used in the prospective ERA, especially of pesticides.

Project objective 1: Model integration

The Cefic-funded project Chimera (http://www.cefic-lri.org/projects/38/21/LRI-ECO19-RUG-ChimERA) aims to address ERA's key challenges, as outlined above, by advancing mechanistic exposure and effect models and integrating them into one predictive modelling framework. The first main objective of this project is therefore to couple separate exposure and effect models (here called 'sub-models') into a chemical-integrated exposure and effect ecosystem model for ecological risk assessment for the aquatic environment (ChimERA, Fig. 1). This will be realised by combining expertise on chemical fate and exposure modelling (University of Insubria, Italy), and effects modelling on the level of individuals, populations and ecosystems (Alterra, Ghent University and Namur University). Just as the mythological Chimera is a creature composed of parts of various animals (http://en.wikipedia.org/wiki/Chimera_(mythology)), our project will integrate ERA's building blocks into one predictive tool that will be subject to extensive testing using data from dedicated experimental work and from existing experiments performed with model ecosystems and using uncertainty and sensitivity analyses.

Developing a robust and predictive integrated model for ERA is a complex and time-consuming task. We will therefore use existing sub-models as much as possible, focus on a spatial network of lentic aquatic ecosystems (e.g. slow streaming ditches, ponds, lakes) containing primary producers, detritus and invertebrates (grazers, detritivores and predators), exposed to (mixtures of) 'model chemicals', including plant protection products and aromatic hydrocarbons. In addition, this project will initiate a 'tiered' approach to model development, i.e. ChimERA will include stylized, simplified representations, which can be replaced by more complex modules in future efforts. For example, ChimERA will use toxicokinetic/toxicodynamic (TK/TD) sub-models to assess internal exposure and effects on survival (Jager et al. 2011). Thus, ChimERA will already be useable in ERAs for

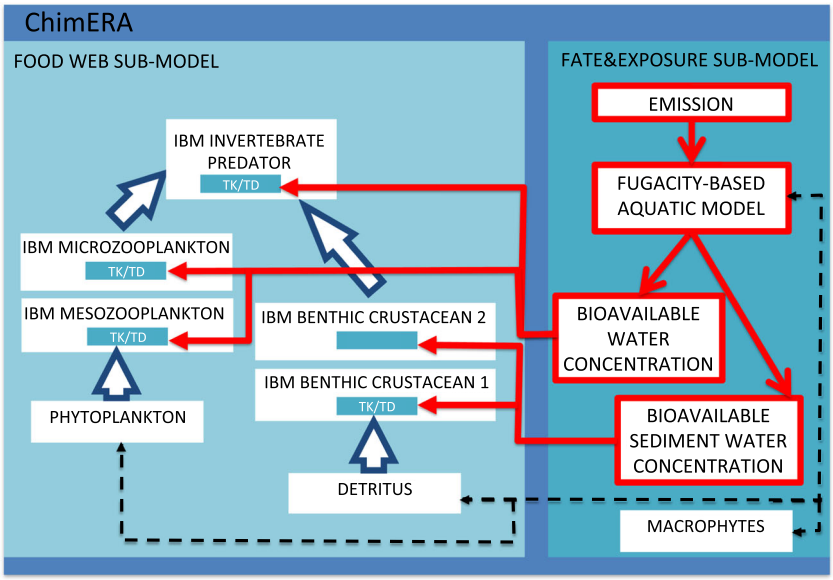

Fig. 1 Structure of the integrated ERA model 'ChimERA', composed of sub-models for chemical fate and exposure, and individual (TK/TD), population (IBM) and community-level (food web model) effects. *Red arrows* contaminant fluxes, *white arrows* mass/individual flows and *black dashed lines* dependence during computation

chemicals for which these effects dominate. Nevertheless, should certain chemicals or applications require so, more detailed alternatives, such as Dynamic Energy Budget sub-models (Martin et al. 2013), can replace the TK/TD sub-models in ChimERA, e.g. to simulate effects on energy allocation and use, and herewith on, e.g. growth and reproduction. By design, ChimERA can therefore be adapted to assess risks for many aquatic ecosystems, exposed to many stressor types. Thus, ChimERA is best described as a prototype, which can already be used, but its main mission is to serve as a proof of concept and initiate further work to meet the challenges listed above using a scientifically underpinned approach.

Project objective 2: Model testing

Whether or not models will be given full consideration as a tool for ERA is to a large extent determined by their transparency and accuracy. In particular, (1) it needs to be clear how the model is structured; (2) sub-models should be tested to prevent the integrated model being correct for the wrong reasons; (3) the main behaviour of the model should be well understood; (4) the model's capacity to predict patterns of exposure and effects observed in natural or semi-natural systems needs to be demonstrated (see Augusiak et al. 2014 for a thorough discussion). We propose two testing approaches: one that is focused on the individual sub-models and one that focuses on testing the key linkages between sub-models. The first approach will evaluate, using dedicated experiments, if the key processes of exposure and effect are well captured by the sub-models in ChimERA. Based on such exercises, differences between data and predictions will be minimised by calibrating parameters of the sub-models that describe these processes. A second approach to model testing will use available semi-field data to evaluate whether the integration of all key processes into ChimERA, i.e. the integrated model containing all sub-models, results in predictions that are sufficiently accurate for environmental decision-making. The testing and calibration phases performed to achieve model testing will rely on the TRACE documentation framework (Schmolke et al. 2010), which recently was proposed to address all questions regarding transparency in a standardised way. To evaluate accuracy, we will use 'pattern-oriented modelling', a multi-criteria design, testing and parameterization approach for ecological models (Grimm et al. 2005). In this approach, multiple patterns observed in the real system (at different scales and levels of organisation) are used to evaluate model predictions, showing which aspects of reality are captured well by the model and which are not and thus require more work.

Project objective 3: Model application

The aim of this project is not to collect an extensive amount of new data but to produce new knowledge by making optimal use of existing data, mechanistic modelling and a limited set of dedicated experimental work. This project will provide risk assessors with a simulation tool to quantify exposure, effects and recovery for predefined environmental conditions and scenarios. Therefore, a third objective of the project is to demonstrate how ChimERA can help to identify those environmental and ecological conditions where risk is expected to be highest. To this end, an extensive scenario analysis will simulate exposure and effects of chemicals and their mixtures in the considered lentic ecosystems, located in a large array of different hypothetical landscapes, representing the range of environmental conditions found in the EU surface waters. By

comparing the effects among the various conditions, we will be able to identify those conditions for which risk is highest. Thus, these results can assist in identifying the environmental scenarios most vulnerable for chemical toxicity.

Project objective 4: Stakeholder involvement

The project aims to initiate a paradigm shift in the approaches used to assess risk of chemicals in aquatic ecosystems. We feel that such an initiative can only be successful when collaborating with potential stakeholders. Therefore, it is important to actively involve these parties through a series of workshops, the first of which was held at Ghent University (27–28 November 2013). During this workshop, it was discussed how ChimERA could advance ERA, but also what the main pitfalls are of using models in risk assessment. During a second workshop (planned in 2015), three main topics will be covered. As a first topic, we will discuss the implications of our scenario analyses for ERA practice. A second topic focuses on the translation of the risk predicted by ChimERA to measures of risk that can be readily used in a regulatory ERA context. Lastly, because ChimERA will be open to include an unlimited number of additional processes to further increase its mechanistic basis, a third topic will include potential future extensions in the context of stakeholders' needs and expectations.

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