EU-Projects

MODELKEY

Models for assessing and forecasting the impact of environmental key pollutants on freshwater and marine ecosystems and biodiversity

Werner Brack[1]*, Joop Bakker[2], Eric de Deckere[3], Charlotte Deerenberg[4], Jos van Gils[5], Michaela Hein[1], Pavel Jurajda[6], Bas Kooijman[7], Marja Lamoree[7], Sovan Lek[8], Maria Jose López de Alda[9], Antonio Marcomini[10], Isabel Muñoz[11], Silke Rattei[1], Helmut Segner[12], Kevin Thomas[13], Peter Carsten von der Ohe[1], Bernhard Westrich[14], Dick de Zwart[15], Mechthild Schmitt-Jansen[1]

[1] UFZ Centre for Environmental Research, Permoserstraße 15, 04318 Leipzig, Germany
[2] National Institute for Coastal and Marine Management / RIKZ, Kortenaerkade 1, 2500 EX 's-Gravenhage, The Netherlands
[3] University of Antwerp, Universiteitsplein 1, 2610 Wilrijk, Belgium
[4] Netherlands Institute for Fishery Research (RIVO), Wageningen UR, POB 68, 1970 AB, IJmuiden, The Netherlands
[5] DELFT Hydraulics, Rotterdamseweg 185, 2600MH Delft, The Netherlands
[6] Institute of Vertebrate Biology, Academy of Sciences of the Czech Republic, 60365 Brno, Czech Republic
[7] Vrije Universiteit Amsterdam, De Boelelaan 1087, 1081 HV Amsterdam, The Netherlands
[8] Centre National de Recherche Scientifique – Midi Pyrenees, 14-16 Avenue Edouard Belin, 31055 Toulouse, France
[9] Chemical and Environmental Research Institute of Barcelona, Jordi Girona, 18-26, 08034 Barcelona, Spain
[10] Consorzio Venezia Ricerche, Via della Libertà 5/12, Marghera, 30175 Venezia, Italy
[11] University of Barcelona, Av. Diagonal, 645, 08028 Barcelona
[12] University of Berne, Laenggass-Straße 122, 3012 Berne, Switzerland
[13] Norwegian Institute for Water Research (NIVA), Brekkeveien 19, POB 173, Kjelsaas, 0411 Oslo, Norway
[14] University of Stuttgart, Pfaffenwaldring 61, 70550 Stuttgart, Germany
[15] Laboratory for Ecological Risk Assessment, National Institute for Public Health and the Environment, A. van Leeuwenhoeklaan 9, 3720 HA Bilthoven, The Netherlands

* **Corresponding author** (werner.brack@ufz.de)

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Abstract

Background. Triggered by the requirement of Water Framework Directive for a good ecological status for European river systems till 2015 and by still existing lacks in tools for cause identification of insufficient ecological status MODELKEY (http://www.modelkey.org), an Integrated Project with 26 partners from 14 European countries, was started in 2005. MODELKEY is the acronym for 'Models for assessing and forecasting the impact of environmental key pollutants on freshwater and marine ecosystems and biodiversity'. The project is funded by the European Commission within the Sixth Framework Programme.

Objectives. MODELKEY comprises a multidisciplinary approach aiming at developing interlinked tools for an enhanced understanding of cause-effect-relationships between insufficient ecological status and environmental pollution as causative factor and for the assessment and forecasting of the risks of key pollutants on fresh water and marine ecosystems at a river basin and adjacent marine environment scale. New modelling tools for risk assessment including generic exposure assessment models, mechanistic models of toxic effects in simplified food chains, integrated diagnostic effect models based on community patterns, predictive component effect models applying artificial neural networks and GIS-based analysis of integrated risk indexes will be developed and linked to a user-friendly decision support system for the prioritisation of risks, contamination sources and contaminated sites.

Approach. Modelling will be closely interlinked with extensive laboratory and field investigations. Early warning strategies on the basis of sub-lethal effects *in vitro* and *in vivo* are provided and combined with fractionation and analytical tools for effect-directed analysis of key toxicants. Integrated assessment of exposure and effects on biofilms, invertebrate and fish communities linking chemical analysis in water, sediment and biota with *in vitro*, *in vivo* and community level effect analysis is designed to provide data and conceptual understanding for risk arising from key toxicants in aquatic ecosystems and will be used for verification of various modelling approaches.

Conclusion and Perspective. The developed tools will be verified in case studies representing European key areas including Mediterranean, Western and Central European river basins. An end-user-directed decision support system will be provided for cost-effective tool selection and appropriate risk and site prioritisation.

Keywords: Artificial neural networks; bioavailability; biofilms; biomarkers; decision support system; effect models; effect-directed analysis; EU-Projects; exposure models; fish communities; *in vitro* tests; invertebrate communities; MODELKEY

1 The MODELKEY Project

MODELKEY is an international research project funded by the European Commission Directorate-General within the Sixth Framework Programme, Priority Global Change and Ecosystems. The project aims to contribute to the assessment, understanding and prediction of the impact of environmental toxicants on aquatic systems at different levels of organisation (from cell to ecosystem), to the development of exposure and effect models, to the assessment and management of contaminated sediments, and to risk assessments on different scales.

MODELKEY is inspired by the demands of the Water Framework Directive (WFD) for a good ecological status of European surface waters by 2015. The WFD demands for a good ecological status of European surface waters by 2015. It focuses on freshwater ecosystems. However, since contaminated rivers are considered major sources of marine pollution, the implementation of the WFD will at the same time make an important contribution to the protection of marine ecosystems. This was decided e.g. in the OSPAR Convention for the North-East-Atlantic and the Barcelona Convention on the Protection of the Mediterranean Sea. The protection of biodiversity (good ecological status) plays a key role in the WFD and in other international and European efforts to protect aquatic environments. It is also the major goal of the Convention on Biological Diversity.

One of the driving forces behind changes in biodiversity is chemical stress due to environmental pollutants. The WFD qualifies the status of aquatic ecosystems based on traditional hydromorphological, physico-chemical and biological parameters, and on priority pollutant concentrations. This procedure allows a rough quality assessment. However, the development of management options, preventive policies and remedial activities requires scientifically sound diagnosis and forecasting of the impact of environmental pollution on freshwater and marine ecosystems. Such diagnosis and forecasting are impeded by many open questions. MODELKEY addresses these questions.

2 Objectives

MODELKEY uses a multidisciplinary approach that aims at developing interlinked and verified diagnostic and predictive modelling tools as well as state-of-the-art effect-assessment and analytical methods generally applicable to European freshwater and marine ecosystems. The project has the following objectives:

- to assess, forecast, and mitigate the risks of traditional and recently evolving pollutants on aquatic ecosystems and their biodiversity at a river basin and adjacent marine environment scale,
- to identify site- and basin-specific key toxicants, which are not necessarily currently monitored 'priority pollutants',
- to provide a better understanding of cause-effect relationships between the impact of environmental pollution as a causative factor and changes in biodiversity and the ecological status, as addressed by the Water Framework Directive (WFD),
- to provide early warning strategies on the basis of sublethal effects measured *in vitro* and *in vivo* and to provide links to effects on biotic community health and biodiversity,
- to provide methods for state-of-the-art risk assessment and decision support systems for the selection of the most efficient management options to prevent adverse effects on biodiversity and to prioritise contamination sources and contaminated sites,
- to strengthen the scientific knowledge on an European level in the field of impact assessment of environmental pollution in aquatic ecosystems and biodiversity by extensive training activities and knowledge dissemination to stakeholders and the scientific community.

3 Approach

Chemical pollution is a well known factor that may cause a decline in biodiversity in freshwater and marine ecosystems. However, the diagnosis, prediction and forecasting of toxic impacts demands for a discrimination from other stresses and for reliable cause-effect relationships between chemical pollution and biodiversity decline. To date, no generally accepted approach exists to establish this link between exposure of freshwater and marine ecosystems to environmental toxicants and observable effects on these ecosystems. There are basically two approaches for cause-effect linkage: (1) the deterministic approach that focuses on an understanding of functions, processes and mechanisms and (2) the stochastic approach focusing on an identification of relationships by statistical means. For both approaches MODELKEY will develop innovative and integrative models and experimental tools.

3.1 Deterministic approach

There are still big gaps in understanding links (i) between chemical quality of sediments and surface waters and measurable toxic effects, (ii) between measurable toxicity in *in vivo* and *in vitro* bioassays and effects on higher levels of biological organisation, including population, community and ecosystem and (iii) between the exposure to toxicants at a contaminated site and the exposure on a basin and adjacent coastal area scale.

3.1.1 Link between chemical quality and toxicity

Effect analysis. There is increasing evidence that effect analysis using well designed batteries of *in vitro* and *in vivo* assays can be a powerful tool to discriminate toxicity from other possible causes of biodiversity decline by identifying modes of action and establishing concentration-response relationships. Assays may therefore serve as an early warning that identifies potential hazards before a decline of biodiversity is observed (Schweigert et al. 2002, Vondráček et al. 2004). MODELKEY will strengthen this approach by the development, advancement, standardisation and compilation of tiered panels of bioassays designed for the detection of major effects and optimised with respect to their ecotoxicological and analytical significance, discriminative power, throughput, reproducibility, minimised test volumes and costs. These assay panels do not only serve as early warning tools, but also as primary site characterisation and toxicity identification.

Effect-based identification of key toxicants. To date, chemical quality assessment is based on chemical analysis of priority pollutants as laid down in the WFD. About 60 compounds have been selected as priority pollutants in different priority categories. To date, about 16 million compounds are known and registered in the Chemical Abstracts (CAS), indicating a tremendous discrepancy between the number of compounds potentially present in the environment and the number of regularly monitored priority pollutants. Numerous studies combining chemical and biological approaches to hazard assessment of complex environmental mixtures indicate that priority pollutant concentrations are a poor indicator of toxicity (Jacobs et al. 1993, Hollert et al. 2005). Thus, it is evident that the aim identified in the Sixth Framework Programme by the European Commission to assess and forecast the impact of chemical pollution cannot be met on the basis of priority pollutant analysis alone. It demands an effect-based identification of key toxicants that are responsible for measurable effects (Brack 2003, Thomas et al. 2004). MODELKEY will address this demand (a) by providing a toolbox for effect-directed analysis (EDA) including a basic set of generally accessible, standardised and comparable EDA methods for European-wide use, (b) by developing innovative and tailored tools for addressing those problems which cannot be solved by existing EDA methods, e.g. the fractionation and identification of compounds generally occurring in very complex mixtures of isomers such as polyaromatic compounds, (c) by establishing a comprehensive and generally accessible key toxicant database including toxicological, physico-chemical, and spectroscopical properties that help to facilitate EDA on an European scale, (d) by training of scientists from different parts of Europe and dissemination of tools and results in order to promote EDA for a better impact assessment in European basins, and (e) by identifying key toxicants in basins selected for case studies in MODELKEY.

Assessment of bioavailability and food chain accumulation. There is increasing evidence that bioavailable fractions rather than total concentrations of chemicals in aquatic ecosystems determine the exposure of biota to toxicants (Adams et al. 1992, Kukkonen et al. 2004). For persistent lipophilic organic toxicants and heavy metals the accumulation in the food web also plays an important role (Morrison et al. 1997). Thus, MODELKEY will provide innovative and powerful tools and approaches for addressing bioavailability and food chain accumulation including (a) properly calibrated and verified state-of-the-art food chain models, (b) tissue extraction and analysis of internal concentrations in test and field organisms and relating them to observed effects, (c) identification of key factors determining the bioavailability of sediment- and suspended matter-associated toxicants, and (d) derivation of the primary target species of those toxicants. The food chain model will be integrated as innovative module into integrated exposure models.

3.1.2 Link between in vitro and in vivo toxicity and effects on higher levels of biological organisation

While bioassays are powerful tools for diagnostic purposes on a cellular and organism level, our understanding of effect propagation on populations, communities and ecosystems is still rather limited. MODELKEY addresses this problem with innovative theoretical concepts supported by modelling tools and with diagnostic laboratory and field tools for assessing effects on species, populations, and communities. A modelling approach based on the concept of dynamic energy budgets (DEBs) using canonical communities and simplified food chains will be used for a better understanding of effects on communities and trophic levels (Kooijman 2000). Model results will be linked to laboratory experiments and field assessment, which focus on the same endpoints relevant to DEBs. Experimental assessment of effect propagation will focus on finding links between toxicity to cells *in vitro*, and organisms *in vivo*, and community effects. State-of-the-art concepts focused on in MODELKEY include pollution-induced community tolerance (PICT) (Schmitt-Jansen & Altenburger, 2005a), microcosm-approaches (Schmitt-Jansen & Altenburger 2005b), and *in situ* biomarkers (Behrens & Segner 2005, Kammann et al. 2005). Effects on biodiversity are assessed on the basis of metabolic profiling (Robertson 2005), taxonomic analysis (Wolfram et al. 2002) and integrative ecological indexes (De Pauw & Heylen 2001) on the one hand and important functional parameters such as photosynthesis, reproduction and growth rates on the other (Guasch et al. 2003).

3.1.3 Link between sites and basins

While exposure to key toxicants may be experimentally determined at a site scale, at a basin scale exposure modelling is believed to be the most efficient way to predict the large scale chemodynamics of contaminants (Baart et al. 2003). Easy to use generic exposure models for risk assessment of contaminated sediments, which provide good predictions with a limited number of input parameters and which take into account the major processes relevant for risks to downstream ecosystems are still to be developed. This will be done by MODELKEY with specific focus on erosion and sedimentation processes, transport and fate of contaminants and food chain accumulation. Extensive model calibration and verification by innovative experimental tools will be performed.

3.2 Stochastic approach

With respect to the development of management strategies for safeguarding of biotic integrity, there is a big demand for tools allowing an attribution of most probable causes to overall effects even without fully understanding the highly complex interactions within an ecosystem and between an ecosystem and environmental pollution. Thus, MODELKEY wants to provide new stochastic approaches for the identification of probable cause-effect relationships on the basis of large data sets on chemical pollution, habitat, toxicity and biological inventories. This will include integrated diagnostic models for the identification of probable causes as well as component models for the prediction of effects of individual toxicants and mixtures on biodiversity. Diagnostic models comprise bioavailability considerations, RIVPACS-type modelling (River Invertebrate Prediction and Classification System), species sensitivity distribution (SSD) statistics, rules for mixture toxicity evaluation, regression techniques, classification techniques, and regression trees (Wright et al. 2000, Posthuma et al. 2002). Predictive component models include classical statistical approaches as well as modern statistics like artificial neural networks (Park et al. 2003). GIS-based analysis of integrated risk indexes will be provided and linked to an end-user friendly decision-support system (DSS) that will help environmental managers to prioritise risks and measures. This will be extremely helpful in the development of cost-efficient management options, remedial action strategies, and preventive policies aimed at mitigating harmful effects on ecosystems and their biodiversity (Critto et al. 2002). A close collaboration with environmental and water agencies that are responsible for monitoring activities and the implementation of the WFD will provide a quick exchange of data, scientific results and requirements between MODELKEY and the end users of MODELKEY results.

4 Project Structure

MODELKEY is organised in 7 subprojects (**Fig. 1**):

- KEYTOX (lead: Kevin Thomas) aims at the development and application of tools to identify effect-directed site- and basin-specific key toxicants (including state-of-the-art effect assessment and analytical methods). These key toxicants are instrumental in the establishment of cause-effect relationships and improved risk assessment.
- BASIN (lead: Eric de Deckere) will compile existing data and insert new monitoring data collected during the MODELKEY project into a database that will be linked to other databases. The database will be the basis for site selection and basin-directed impact assessment.
- EXPO (lead: Jos van Gils) will focus on the establishment of easy-to-use exposure models to predict risks of toxic pollution in river basins and adjacent coastal areas. The models will include modules on most relevant processes, including sediment erosion and sedimentation, transport and fate, and bioavailability and food web accumulation.
- EFFECT (lead: Sovan Lek) aims to develop deterministic and stochastic models to understand, diagnose and predict the effects of pollutants on populations, communities and ecosystems.
- SITE (lead: Mechthild Schmitt-Jansen) will deliver and apply site-directed experimental laboratory and field tools to determine processes, cause-effect relationships and effect propagation. SITE focuses on providing a better understanding of the toxic impact on aquatic ecosystems and on calibration and verification of the modelling tools. SITE will also apply innovative early warning systems such as *in vitro* assays and biomarkers.
- DECIS (lead: Antonio Marcomini) aims at developing integrated risk indices and decision support systems exploiting MODELKEY results to improve management, preventive policies and cost-efficient remedial activities.
- TRAIN (lead: Joop Bakker) will organise training programmes for MODELKEY participants, external scientists and end-users.

All subprojects are implemented in three different river basins including their estuary and coastal zone. The Llobregat (Spain) is a typical Mediterranean river basin; the Elbe (Czech Republic, Germany) and its catchment area represents a large central European river basin; and the Scheldt and its tributaries (France, Belgium, The Netherlands) are a relatively small western European river system. These freshwater ecosystems receive significant pollution from point and diffuse sources, including present and former industrial production, municipal wastewater treatment plants and agricultural production.

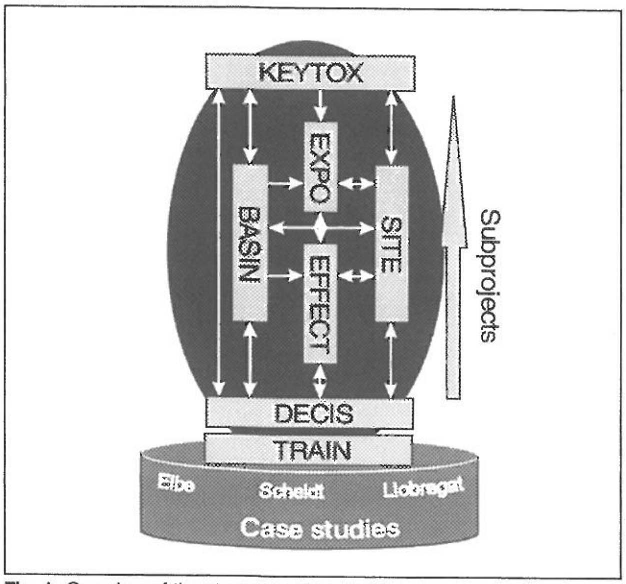

Fig. 1: Overview of the structure of the project

Project co-ordination (Werner Brack, Mechthild Schmitt-Jansen) and management (Michaela Hein, Silke Rattei) are done by the UFZ Centre for Environmental Research in Leipzig, Germany.

5 The MODELKEY Consortium

The MODELKEY consortium consists of 26 partners from 14 European countries (**Table 1**). It comprises scientific groups with experience in effect-directed analysis, in fish, invertebrate, and microbial ecology and ecotoxicology, in environmental chemistry and analysis, in sediment hydraulics, in exposure, effect and risk modelling, in socio-economic assessment, as well as in the design of decision support systems. Important end-users of MODELKEY results, e.g. agencies that are responsible for river basin management and the implementation of the Water Framework Directive, are either included in the consortium itself or involved in a specific MODELKEY end-user communication board. This board is designed to organise the quick exchange of requirements, ideas, and data between different end-users as well as end-users and MODELKEY scientists.

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Table 1: The MODELKEY consortium

Project partner	Short name	Country	Key Scientists
UFZ Centre for Environmental Research	UFZ	Germany	Werner Brack, Mechthild Schmitt-Jansen, Peter von der Ohe
University of Antwerp	UA	Belgium	Eric de Deckere
Centre for Environment, Fisheries, and Aquaculture	CEFAS	United Kingdom	Jan Balaam
WL| Delft Hydraulics	DELFT	The Netherlands	Arthur Baart, Jos van Gils
Consorzio Venezia Ricerche	CVR	Italy	Antonio Marcomini
Vrije Universiteit Amsterdam	VUA	The Netherlands	Bas Kooijman, Marja Lamoree, Bert van Hattum
Centre Nationale de Recherche Scientifique – Midi-Pyrénées	CNRS	France	Sovan Lek
Chemical and Environmental Research Institute of Barcelona – Spanish Council for Scientific Research	CSIC	Spain	Miren López de Alda, Damià Barceló
Universitat de Girona	UdG	Spain	Sergi Sabater
University of Berne	UB	Switzerland	Helmut Segner
Veterinary Research Institute	VRI	Czech Republic	Miroslav Machala
Institute of Vertebrate Biology	IVB	Czech Republic	Pavel Jurajda
University of Joensuu	UJOE	Finland	Jussi Kukkonen
Elbe Water Quality Monitoring Agency	ARGE Elbe	Germany	Thomas Gaumert
National Institute for Coastal & Marine Management	RIKZ	The Netherlands	Joop Bakker
Netherlands Research Institute for Fisheries Research	RIVO	The Netherlands	Pim Leonards, Charlotte Deerenberg
Slovak Medical University	SZU	Slovakia	Anton Kočan
The Netherlands National Institute for public Health and the Environment	RIVM	The Netherlands	Dick de Zwart
University of Stuttgart	UoS	Germany	Bernhard Westrich
Saint-Petersburg State University	SPbU	Russia	Vladimir Nikiforov
University of Barcelona	UdB	Spain	Isabel Muñoz
Catalan Water Agency	ACA	Spain	Antoni Ginebreda
ECT Oekotoxikologie GmbH	ECT	Germany	Thomas Knacker
Xenometrix by Endotell GmbH	XEN	Switzerland	Sini Flückiger
Donabaum&Wolfram OEG	DW/OH	Austria	Georg Wolfram, Claus Orendt
Norwegian Institute for Water Research	NIVA	Norway	Kevin Thomas

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