# SETAC Europe 20th Annual Meeting
## 23-27 May 2010, Seville, Spain
## LIST OF SHORT COURSES

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## SHORT COURSE 1: Use of QSAR models for REACH: practical use of the CAESAR models

**Instructors:**
Elena Boriani (Mario Negri Research Institute, Italy), Emilio Benfenati (Mario Negri Research Institute, Italy)

**Course length:**
Half day (8.00-12.00 hrs)

**Course level:**
Introductory

**Description:**
REACH is the new European Community Directive on chemicals and their safe use protecting the human health and the environment. To supply the necessary information, the existing data are not enough. In order to reduce the number of animal tests, the REACH legislation establishes and promotes the use of alternative methods, like in-silico methods. By using non-testing methods, it is possible to reduce the number of animal tests and the costs of the tests. Within the CAESAR EU project (www.caesar-project.eu) specific in-silico models for REACH endpoints have been developed to predict the biological activity of the chemicals. This course provides a practical overview of the so-called "non-testing methods", their main characteristics and possible applications, focusing on CAESAR models and other ones. There are models based on the interpolation of the existing data of similar compounds and some, like CAESAR, where the missing property (physicochemical, toxicological or ecotoxicological properties) is predicted on the basis of the chemical structure. Moreover, with QSAR it is possible to proceed in batch, testing many compounds at the same time. This course is strongly recommend to understand the meaning of QSAR model results and critically and correctly interpreting in the contest of chemical safety for REACH.

**Objectives:**
The course will provide an introduction to the use of alternative methods, in particular QSAR, for assessing chemical properties and toxicity data for REACH compounds. CAESAR models and other comparative applications will be tested and results will be critically discussed. The course is not aimed to teach all QSAR features but recommended practices to deal with in silico methods in a critical way.
Participants will understand the basic concepts of models built to predict properties and toxicity endpoints, being able to perform their own calculation using the user friendly, freely available CAESAR models and interpret the obtained results.

**Course outline:**

08.00 - 08.15     Introduction to alternative methods requirements for REACH legislation
- REACH legislation
- REACH requirements
- Alternative methods

We will introduce the approach given by the REACH legislation on the QSAR methods. The requirements for these methods are defined by REACH. We will compare the European approach with the approach used in the USA.

08.15 - 09.45     Brief introduction on QSAR methods
- How to build up a reliable model (Theoretical aspects, training data, OECD principles, accuracy, sensitivity, specificity)
- Main characteristics of a QSAR model
- Applicability domain
- False positives – False Negatives

We will introduce the theoretical basis of the QSAR methods, defining the different modes, such as classifiers and regression methods. The chemical information will be described, and the use of the different descriptors. We will show the ways to assess performance of the models. The specific requirements of REACH will be illustrated with practical examples. Pitfalls of the QSAR methods will be shown, and tools to assess the applicability domain of the models. We will describe the different QSAR philosophies, and existing solutions adopting diverse approaches. Links to QSAR models will be listed. We will introduce the basic operative procedure on how to use

simple models.

*09.45 - 10.00*   *Coffee break*

10.00 - 10.30   Endpoints treated with CAESAR models
- Why these endpoints? Main characteristics of each endpoint - model features - applicabilities
- BCF
- Skin Sensitisation
- Mutagenicity
- Cancerogenicity
- Developmental Toxicity

We will shortly present the five endpoints and the results obtained, using the validation sets for the assessment of these models.

10.30 - 11.30   QSAR CAESAR model, practical use
- User Inputs (structures – batch files – formats – converter)
- Applicability domain
- Calculation of various examples
- Critical Analysis of results obtained
- Applications / Future Uses

Students will be trained to the use of European and USA freely available models. The way to introduce the chemical structure will be shown. The practical ways to obtain results will be described, and commented. Properties of interest will include ecotoxicity values, and bioconcentration factors.

11.30 - 12.00
- Comparison within experimental values /other software results
- Understanding the meaning behind a QSAR approach
- Review, questions and course evaluation

We will summarise the main lessons and the advantages and disadvantages of the methods. Questions will be addressed.

## Products / course materials:
Reprints of relevant published articles, handouts of lecture slides and other course materials including files of the calculated examples and interesting and useful links.

## Participants to bring their own laptop to the course:
Yes

**Instructors:**
Tom Hutchinson (Cefas, UK), Tony Millais (Cefas, UK), David Sheahan (Cefas, UK)

**Course length:**
Half day (13.00-17.00 hrs)

**Course level:**
Introductory

**Description:**
It is recognised internationally that risk assessment approaches for chemicals need to consider potential impacts on marine environments. Both the European Commission report on legislation in the area of chemicals (including agrochemicals, biocides, industrial chemicals and pharmaceuticals) and the OSPAR Hazardous Substances Strategy recognise the need for marine risk assessment data. Under OSPAR, particular concerns focus on substances that are considered as Persistent, Bioaccumulative and Toxic (PBTs). Global demographic factors leading to major increases of human populations along coastlines, the rapid development of marine technologies and energy production (eg offshore energy generation) and coastal flood risks due to climate change are additional long-term challenges for marine risk assessment. Coastal aquaculture is also increasingly important as a human food source. Against this background, this introductory short course will cover the following key elements: (1) EU, North American and other international policy drivers (eg REACH) for marine risk assessment of chemicals and pharmaceuticals; (2) marine fate assessment including contaminated sediment assessments (3) marine effects assessment case studies – including the OSPAR Offshore Chemicals Notification Scheme (OCNS) for the oil and gas sector plus a pharmaceutical case study; and (4) current global challenges in marine risk assessment across Europe, North America and south-east Asia.

**Objectives:**
(1) To provide participants with an introduction to marine pollution issues and the need for marine risk assessments to also consider climate change and demographic impacts on coastal zones;
(2) To give a state-of-the-art review of current marine risk assessment policy drivers pertinent to agrochemicals, biocides, industrial chemicals and pharmaceuticals;
(3) To describe key case studies on the persistence and fate aspect of marine risk assessment as applied to industrial chemicals (eg OSPAR Offshore Chemicals Notification Scheme for the oil and gas sector);
(4) To share experience of marine effects assessment approaches for chemicals and pharmaceuticals, including intelligent testing strategies and optimal marine species selection.

**Course outline:**
13.00 - 13.15  Welcome
13.15 - 14.00  Introduction to marine contamination problems and the cumulative challenges of climate change and demographic pressures on coastal ecosystems. A brief introduction to fundamental concepts in risk assessment will be provided, followed by an overview of the key EU and other regional policy drivers pertinent to marine risk assessment *(Lead instructor - Tom Hutchinson)*;
14.00 - 15.00  Marine Fate & Persistence Assessment. This part of the short course will provide an overview of the abiotic processes (eg hydrolysis, phototransformation, etc) and biotic processes (including ready and ultimate biodegradation) pertinent to evaluating the fate of chemicals and pharmaceuticals in marine systems. Modelling tools for predicting exposure concentrations (deriving the $PEC_{marine}$) will be presented (eg CHARM and DREAM models as used for Offshore Chemical Notification Schemes in Europe *(Lead instructor - Tony Millais)*;
*15.00 - 15.15  Coffee break*
15.15 - 16.15  Bioconcentration & effects assessments for marine ecosystems. Pragmatic regulatory approaches to measuring and predicting bioconcentration values will be discussed. The principles of deterministic and probabilistic hazard assessments will be presented (deriving $PNEC_{marine}$ and $HC5_{marine}$). The pros and cons of using

freshwater base set data in these assessments will be discussed alongside the growing toolbox of marine ecotoxicology test methods (eg ASTM, ICES, ISO, OECD and US EPA Standard Evaluation Procedures) and how they can be used in a targeted and efficient manner.  Brief consideration will be given to assessing effluents and other complex mixtures, together with marine sediment test methods.  An marine case study of an azole fungicide will be presented *(Lead instructor - Dave Sheahan)*.

16.15 - 16.45  Open discussion (Attendees are encouraged to send questions in advance that can then be included in this discussion session)

16.45 - 17.00  Concluding remarks *(All Instructors)*

**Products / course materials:**
• Course handbook including printouts of all PowerPoint presentations;
• Electronic copies of all course material (to be emailed directly to participants);
• List of key Internet resources to support marine risk assessments of chemicals (in course handbook).

**Participants to bring their own laptop to the course:**
No

**Instructors:**
Matthias Liess (UFZ, Germany), Mira Katwinkel (UFZ, Germany), Mikhail Beketov (UFZ, Germany),

**Course length:**
Half day (13.00-17.00 hrs)

**Course level:**
Introductory

**Description:**
Linking community data and exposure is one of the challenging tasks of environmental risk assessment. For example when using monitoring data for post-registration studies or the interpretation of mesocosm results. The major challenges for this exercise include dealing with (i) confounding factors, (ii) differences in community composition of sample sites and mesocosm replicates and (iii) rare species.
The aim of the course is twofold:
> 1) To inform on the relevant processes that are to be considered when linking community data and exposure.
> 2) To apply the knowledge obtained using a simple spreadsheet calculator, exercising with real data.

Participants will take home a profound knowledge on pitfalls and possibilities in the area of linking community data and exposure. They will also be enabled to independently calculate concentration-response relationships of complex community data.
The instructors have 20 years of experience in linking community data and exposure. They have organised the EU SETAC workshop EPiF on effects of pesticides in the field (http://www.systemecology.eu/EPiF/Download.html), and designed the SPEAR indicator system used to identify and predict effects of pesticides in streams (http://www.systemecology.eu/SPEAR/Start.html).

**Objectives:**
Participants will take home a profound knowledge on pitfalls and possibilities in the area of linking community data and exposure. They will also be enabled to independently calculate concentration-response relationships of complex community data.

**Course outline:**
(1) Participants will be presented a detailed overview on the major challenges when attempting to link community data and exposure. The relevant literature on that topic will be considered.
(2) Based on the challenges presented approaches will be explained on how to overcome the challenges.
(3) With a "hands on" experience participants will be enabled to use a calculator applying the knowledge gained on real data, provided by the instructor. The use of own data is possible as well (contact instructor beforehand to put data in a ready to use format).

13.00 - 13.45    Introduction, overview, discussion
13.45 - 14.45    First half of material
*14.45 - 15.00    Coffee Break*
15.00 - 16.30    Second half of material
16.30 - 17.00    Review, questions and course evaluation

**Products / course materials:**
- Detailed list of major challenges when attempting to link community data and exposure;
- Detailed list of approaches to link community data and exposure;
- Literature review;
- Calculator to perform assessments of own data.

**Participants to bring their own laptop to the course:**
Yes

**Instructors:**
Hans Rufli (ecotoxsolutions, Switzerland)

**Course length:**
Full day (8.00-17.00 hrs)

**Course level:**
Intermediate

**Target audience:**
Candidates interested in the scientific background of advanced aquatic ecotoxicological testing procedures. Basic background knowledge on aquatic ecology and ecotoxicological testing is considered necessary.

**Description:**
The course provides guidance on how to perform algae-, daphnia- and fish-tests taking into account the recent changes in EU regulations, US-EPA test- and OECD technical Guidelines, and how to produce scientifically valid studies accepted by the authorities in the EU, US and Japan. Each test method is exemplified with reactions of the authorities to studies submitted showing why authorities declared that a particular study did not satisfy the guideline requirements.
The course further provides information on the philosophy of testing and its background beyond what is stated in the guidelines, on effect-concentration and time-concentration relationships, on extrapolations from results of acute to chronic tests and from laboratory test results to the environment.
Last but not least, guidance will be given on how to best interpret and report studies. A case study based on an acute fish test with a 'difficult to test substance' will illustrate reporting needs and deficiencies. Examples will be discussed on how to best report results of aquatic ecotoxicology studies.

**Objectives:**
The course provides guidance on testing methods and strategies in aquatic ecotoxicology. It provides the knowledge and skills to optimise the testing in order to avoid the production of invalid data and the repetition of studies.

**Course outline:**
08.00 - 08.30   General Introduction: Introduction of participants, illustration of objectives, distribution of handouts.
08.30 - 09.15   Successful Testing of Fish including Case Studies with Reactions of the Authorities: Guidance on how to perform the tests, optimal conditions for test organisms, how to produce scientifically valid studies accepted by the authorities in the EU, US and Japan.
09.15 - 09.45   Successful Testing of Daphnia and Algae: Guidance on how to perform the tests, optimal conditions for test organisms, how to produce scientifically valid studies accepted by the authorities in the EU, US and Japan.
*09.45 - 10.00   Coffee break*
10.00 - 10.30   Successful Testing of Daphnia and Algae continued
10.30 - 12.00   Case Studies of Daphnia and Algae Tests: Reactions of the authorities to specific studies.
*12.00 - 13.00   Lunch*
13.00 - 14.45   Parameters affecting Toxicity: Effects of concentration, period of exposure, sensitivity of endpoints and life stages of fish on the toxicity, acute to chronic ratios.
*14.45 - 15.00   Coffee break*
15.00 - 15.30   Data Reporting: Guidance on a scientifically meaningful expression of toxicity data.
15.30 - 16.15   Case Study on Reporting: List of questions to be discussed.
16.15 - 16.45   Review & questions
16.45 - 17.00   Course evaluation

**Products / course materials:**
Files with handouts.

**Participants to bring their own laptop to the course:**
No

**Instructors:**
Francesco Falciani (University of Birmingham, UK), Tim Williams (University of Birmingham, UK), Ed Perkins (US Army Corps Engineers ERDC, USA), Philipp Antczak (University of Birmingham, UK)

**Course length:**
Full day (8.00-17.00 hrs)

**Course level:**
Introductory

**Target audience:**
Researchers interested in using multi-level large datasets (for example derived from the application of functional genomics technologies)

**Description:**
The development of Functional Genomics technologies (e.g. gene expression profiling, high-throughput sequencing, proteomics and metabolomics) have in recent times increased our capacity to characterize at the molecular level the effects of chemical exposure both in laboratory controlled experiments and in field studies. This unprecedented amount of information however also represents a challenge in terms of data management, analysis and interpretation. In particular, key to the successful integration between investigative approaches and the development of robust markers of interest to regulatory authorities is the integration between field measurements of contamination and environmental impact with organism multi-level molecular measurements. This clearly can only be achieved by extensive use of computational methods.
This course is designed to offer researchers in ecotoxicology a basic but rigorous introduction to the bioinformatics workflow that addresses this important need. In this one day course, the instructors will provide an intuitive level introduction to the methodologies and a series of hands on guided tutorials to solve real world scenarios. The instructors have designed this as an introductory course; therefore no previous training in Bioinformatics will be required. Because of the importance and potential broad impact of these approaches in eco-toxicology it is anticipated that this course will interest both researchers and regulators.

**Objectives:**
The overall objective of the course is to provide participants with an introduction to the analysis techniques used for integration and analysis of these data. More specifically, it is expected that at the end of the course the participants will be able to:
(1) Design experiments and studies that make extensive use of "Omics" techniques. This will involve the use of simple statistics to establish the correct sample size for a study.
(2) Use state-of-the-art but easy-to-use software tools to identify genes/proteins/metabolites differentially expressed in different sample groups.
(3) Use statistical modelling to identify molecular signatures predictive of adverse outcome.
(4) Use pathway inference tools to infer the structure of underlying molecular networks associated to adverse outcome.
(5) Use software tools that facilitate biological interpretation of the results.

**Course outline:**
The focus of the course is in providing an overview of the techniques that can be useful for the identification of predictive markers particularly in relation to questions of ecotoxicological relevance.
This will include the integration of molecular and physiological information in the analysis of laboratory exposures and samples collected from relevant environmental sites. In order to make this possible, the instructors will provide multi-level measurement datasets from an academic (School of Biosciences, University of Birmingham, UK) and a government laboratory (USA Army Corps of Engineers, USA). These datasets will represent both laboratory and field studies.
In addition, the purpose is to enable the course participants to seamlessly transfer the skills and resources (e.g. software) acquired in the course of the tutorials to their own research environments. The instructors intend to achieve this by providing a user-friendly open source software analysis platform based on the BioLinux (http://nebc.nox.ac.uk/tools/bio-linux/bio-linux-5.0) operative

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system. This independent software platform will be accessed by the course participants by booting their own laptops from a USB memory stick that will be provided during the course.

The course will include short theoretical introductory sessions where the basic statistical methodologies will be explained at an intuitive level, followed by hands-on assisted step by step tutorials. The customized version of BioLinux that will be provided to support the course will include the following software applications: 1) TMEV (Exploratory analysis), 2) GALGO (Biomarker discovery), 3) ARACNE (Network inference), 4) Cytoscape (Network, pathway visualization and biological interpretation).

| | |
|---|---|
| 08.00 - 08.15 | Introduction and overview |
| 08.15 - 08.45 | Experimental Design |

08.15 - 08.45    Experimental Design
A brief theoretical overview of the issues behind designing laboratory exposure and field studies based on large-scale multi-level measurement platforms. Two case studies will be presented.

08.45 - 09.45    Exploratory analysis and identification of interesting variables
A hands-on overview of the basic exploratory analysis techniques (Cluster analysis and Principal Component Analysis) which allow the visual representation of the relative similarity of biological samples on the basis of their combined molecular and physiological state. In addition, the basic techniques for identifying interesting variables (e.g. differentially expressed genes, proteins and metabolites) will be shown.

*09.45 - 10.00*    *Coffee break*

10.00 - 11.30    Software assisted biological interpretation of gene lists and pathway mapping techniques
A demonstration of the bioinformatics methods employed to facilitate biological interpretation of the lists of differentially expressed genes obtained in the previous tutorial.

11.30 - 12.00    Discussion and general questions

*12.00 - 13.00*    *Lunch*

13.00 - 13.30    Development of molecular biomarkers predictive of adverse outcome
A brief theoretical overview on statistical modelling with a view to introduce the concept of predictive biomarker.

13.30 - 14.30    Identifying transcriptional signatures predictive of environmental exposure: A case study
A hands-on tutorial on the identification of biomarkers predictive of adverse outcome.

*14.30 - 14.45*    *Coffee break*

14.45 - 15.15    Inferring biological networks from experimental data
A brief theoretical overview on network inference.

15.15 - 16.15    A case study on network inference
This tutorial will introduce a simple network inference technique and its application to reconstruct a biological network representing an important toxicity mechanism.

16.15 - 16.45    Student questions

16.45 - 17.00    Course evaluation

**Products / course materials:**
- The course will be delivered on USM memory devices implementing BioLinux software platform. This solution will enable the course participants to plug the device in their laptop and work through the entire course. Later they will have the option to install all software and datasets on their computers permanently.
- In addition, the course participants will receive printed documentation of the course material, covering the theoretical overview of the methodology and the step-by-step tutorials.

**Participants to bring their own laptop to the course:**
Yes

## SHORT COURSE 7: Statistical methods in ecotoxicology using R

**Instructors:**
Christian Ritz (University of Copenhagen, Denmark), Jens C. Streibig (University of Copenhagen, Denmark)

**Course length:**
Full day (8.30-17.30 hrs)

**Course level:**
Advanced

**Target audience:**
PhD students, researchers and scientists in toxicology and environmental sciences. An elementary understanding of statistical concepts (including ANOVA and regression) is a prerequisite.

**Description:**
The open source statistical environment R (http://www.r-project.org) has become the lingua franca of data analysis among statisticians and is also in widespread use in many applied sciences. Many advanced or recent statistical and graphical/visualisation techniques are only available in R. Therefore, it is an extremely powerful all-in-one alternative software to specialised commercial data analysis software currently used by many ecotoxicologists. Moreover, it encourages collaborative and reproducible research.

The focus will be on giving the participants practical experience with the software. The course material will be a blend of introductory lectures on R (before lunch) and case-studies based on real toxicological data, from recent publications in ET&C and elsewhere (after lunch).

ANOVA methods, linear, non-linear regression (including dose-response analysis), and logistic and Poisson regression models will be introduced. There will also be case-studies on more advanced topics such as automation/simulation, hormesis models, mixture modelling, random effects models, analysis of data with non-detects, and time-to-event methods. Expert teachers will provide guidance and assistance throughout the course.

The course is intended for PhD students, researchers, and scientists in toxicology and environmental sciences. An elementary understanding of statistical concepts (including ANOVA and regression) is a prerequisite. Participants are encouraged to bring their own data.

**Objectives:**
(1) Review state-of-the-art statistical methods for analysis of toxicological data
(2) Demonstrate the power of open source statistical software
(3) Provide hands-on experience for standard data analysis (cookbook)
(4) Enable participants to use the software on their own problems (take-home software)

**Course outline:**
08.30 - 08.45   Introduction/Welcome
08.45 - 09.45   Lecture: Installation and introduction to **R** in the context of ecotoxicology
*09.45 - 10.00   Coffee break*
10.00 - 12.00   Lecture: More on **R**'s capabilities: descriptive statistics, ANOVA and regression, graphics
*12.00 - 13.00   Lunch*
13.00 - 15.00   Case studies- part I (interactive session)
*15.00 - 15.15   Coffee break*
15.15 - 17.20   Case studies – part II ( or analysis of participants' own data)
17.20 - 17.30   Course evaluation & Conclusion

**Products / course materials:**
Hand-outs of the lecture notes and course manual (around 100-page booklet) prepared by the instructors. Installation of the open source software R on participants' own laptops.

**Participants to bring their own laptop to the course:**
Yes

## SHORT COURSE 8: Current registration requirements for ecological risk assessment of crop protection products in the EU

**Instructors:**
Peter Dohmen (BASF SE, Germany), Anne Alix (AFSSA, France), Bernhard Gottesbueren (BASF, Germany), Christine Füll (EFSA), Mark Clook (CRD, UK), Martin Streloke (BVL, Germany), Robert Luttik (RIVM, The Netherlands), Theo Brock (Alterra, The Netherlands)

**Course length:**
Full day (9.00-16.10 hrs)

**Course level:**
Introductory - Intermediate - Advanced

**Target audience:**
All those involved or interested in pesticide regulatory and safety issues. Delegates from consultancies, industry and regulatory authorities, who need an introduction and most current update in the area of pesticide regulation are welcome as are scientists, students

**Description:**
This short course will give participants an update on the current European (EU) registration requirements in the field of ecotoxicological risk assessment. It will outline the standard studies necessary for registration as well as how risk assessments are conducted within the various fields of ecotoxicology. The day will be based around the New Regulation (1107/2009) and respective guidance documents. Accordingly, all the different areas - bird and mammals, aquatic, bees, non-target arthropods, soil, non-target plants - will be covered. Standard requirements and also higher tier testing will be addressed.
The short course will be presented by a number of experts in the area of pesticide regulation and risk assessment.

**Course outline:**
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|---|---|
| 09.00 - 09.15 | Introduction (Peter Dohmen) |
| 09.15 - 10.00 | Introduction to exposure assessment (Bernhard Gottesbueren) |
| 10.00 - 10.45 | Aquatic study requirements and risk assessment (Theo Brock) |
| *10.45 - 11.00* | *Coffee break* |
| 11.00 - 11.45 | Bird and mammal risk assessment (Robert Luttik) |
| 11.45 - 12.30 | Risk assessment to bees and other terrestrial Non-target Arthropods (Anne Alix) |
| *12.30 - 14.00* | *Lunch* |
| 14.00 - 14.45 | Soil testing and risk assessment (Mark Clook) |
| 14.45 - 15.15 | EFSA's role in risk assessment (Christine Füll) |
| *15.15 - 15.30* | *Coffee break* |
| 15.30 - 16.10 | Risk management (Martin Streloke) |

**Participants to bring their own laptop to the course:**
No

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## SHORT COURSE 9: MODELKEY DSS: a Weight of Evidence approach for the ecological status evaluation according to WFD requirements

**Instructors:**
Elena Semenzin (Consortium Venice Research (CVR), Italy), Antonio Marcomini (University Ca' Foscari of Venice, and Consortium Venice Research (CVR), Italy), Stefania Gottardo (University Ca' Foscari of Venice, Italy)

**Course length:**
Full day

**Course level:**
Intermediate

**Description:**
Site-specific ecological risk assessment (ERA) is explicitly required by the Water Framework Directive (WFD) to assess the quality of water bodies across Europe. Specific approaches and decision support tools are required for qualifying the assessment and decisional processes, involving experts, stakeholders and authorities. Within the European project MODELKEY, the Consortium Venice Research (CVR) in collaboration with the Netherlands Institute for Public Health and the Environment (RIVM) has adopted a Weight of Evidence (WOE) approach for ecological status classification and evaluation. Specifically, a framework, Multi-Criteria Decision Analysis (MCDA) tools and a Decision Support System (DSS) were developed to collect, normalize and aggregate indicators belonging to different Lines of Evidences (LOE; biology, chemistry, ecology, ecotoxicology and hydromorphology). This course allows the participants to present and discuss their own indicators, to receive a short introduction on multi criteria decision making, to get instructed about the principles of Weight of Evidence approaches for ERA, and to be trained for the application of the MODELKEY DSS to a selected case study. Upon attendance to the course, the participants are expected to be able to critically apply different tools in ERA and to evaluate the results according to WFD requirements (e.g. set up of investigative monitoring).

**Objectives:**
Increasing familiarization with theory and application of tools for supporting the implementation of site-specific ERA according to Water Framework Directive requirements: the Weight of Evidence approach, MCDA analysis and the MODELKEY DSS.

**Course outline:**
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|---|---|
| 08.30 - 08.45 | Introduction of lectures and attendees |
| 08.45 - 09.15 | <u>Theory of Ecological Risk Assessment and Weight of Evidence approach</u> (Elena Semenzin): Introduction to ERA and WoE concepts. |
| 09.15 - 09.45 | <u>Concepts on Multi Criteria Decision Analysis and Fuzzy Logic</u> (Antonio Marcomini): Introduction to MCDA principles and methods + MCDA methods applied within the MODELKEY DSS including Fuzzy Logic. |
| *09.45 - 10.00* | *Coffee break* |
| 10.00 - 10.30 | <u>Short overview of the decision support system named MODELKEY DSS</u> (Elena Semenzin): Brief introduction to the MODELKEY project and its main outcome: the MODELKEY DSS. Description of software objectives and functionalities. |
| 10.30 - 11.30 | <u>The Integrated Risk Assessment (IRA) methodology for ecological status evaluation developed within MODELKEY</u> (Stefania Gottardo): Detailed explanation of the Integrated Risk Assessment (IRA) methodology developed within the MODELKEY project for the assessment of water quality according to WFD requirements. Specifically details on the application of the WoE approach to indicators organisation and the implementation of a Fuzzy Inference System for indicators aggregation is given. |
| 11.30 - 12.00 | Review, student questions |
| *12.00 - 13.00* | *Lunch* |
| 13.00 - 14.00 | <u>Presentation of indicators by each attendee (5-10 min each) [partly homework] and their inclusion in the IRA methodology</u> (interactive) (Elena Semenzin): Participants should briefly present their own indicators (i.e. biological, chemical, ecotoxicological, physico-chemical, hydromorphological indicators developed or |

used by the participants) and will be guided in assigning them to the correct hierarchical level defined by the IRA methodology (a table will be provided in advance).

In the case that the participants will not have indicators to be presented, 10 default indicators will be suggested and presented by the instructors.

14.00 - 14.20 <u>Case study presentation</u> (Antonio Marcomini): Presentation of the case study selected for the MODELKEY DSS application.

14.20 - 14.45 <u>Application of the MODELKEY DSS</u> [exercise] (Stefania Gottardo, Elena Semenzin):
- Intro: the Environmental module of the MODELKEY DSS (5 min)
- Focus on STEP 2 and 3: Selection of indicators and temporal scale of application: (interactive, 20 min)

*14.45 - 15.00*   *Coffee break*

15.00 - 16.00 <u>Application of the MODELKEY DSS</u> [exercise] (Stefania Gottardo, Elena Semenzin):
- Software demonstration: from STEP 4 to 7 of the Environmental module (15 min)
- Visualisation and discussion of the module's results at both basin and site-specific scale (exercise, 45 min)

16.00 - 16.10 <u>Conclusions</u> (Elena Semenzin): Web site, software availability, future developments

16.10 - 16.20 Review, student questions

16.20 - 16.30 Course evaluation

## Products / course materials:
- lectures handouts
- case study material
- background information (e.g. papers, MODELKEY DSS)

## Participants to bring their own laptop to the course:
Yes

**Instructors:**
Manuele Margni (CIRAIG, Canada), Ralph K. Rosenbaum (CIRAIG, Canada), Tom Mc Kone (University of California, USA), Olivier Jolliet (University of Michigan, USA)

**Course length:**
Full day (8.00-17.00 hrs)

**Course level:**
Intermediate

**Target audience:**
Candidates interested in the scientific background of chemical assessment of environmental emissions. Only basic background knowledge on environmental modelling, risk assessment or LCA is considered necessary.

**Description:**
To answer the increasing need of methods assessing the risk of toxic emissions on human health and ecosystems this course provides a practical overview of multimedia chemical fate modeling, multi-pathway human exposure modeling, and estimation of comparative indicators for human health and aquatic ecotoxicological impact. Typical environmental mass balance modeling concepts are explained, like partitioning coefficients, 1st order rate coefficients, mass balances, persistence, and long-range transport. The fundamentals of multipathway models are then presented for human intake via inhalation, drinking water and food. A brief theoretical introduction is also presented to estimate risk-based and disability-adjusted-life-years (DALY)-based effect, as well ecotoxicological effect factors. Finally, straightforward examples are provided from raw data sets to characterisation factors estimates for human health and ecotoxicological impacts using the USEtox model developed by SETAC/UNEP Life Cycle Initiative designed specifically for the comparative assessment of chemical fate, human exposure, and (eco)toxicological impacts. This short course is strongly based on the outcomes of an international project, where six models where compared and harmonized to develop the USEtox model used to calculate recommended characterization of toxic impacts in Life Cycle Impact Assessment.

**Objectives:**
The course aims to an introduction to toxicological risk and impact modelling for assessing chemical emissions in LCA and other comparative applications. Underlying assumption and recommended practices are presented.
Participants should understand the basic concepts of toxic assessment on human health and ecosystem and being able to perform their own assessment using the USEtox model and interpret the obtained results.

**Course outline:**
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| 08.00 - 08.15 | Welcome |
| 08.15 - 08.30 | General introduction (Manuele Margni): Source to damage cause-effect chain relationship and modelling steps. |
| 08.30 - 09.45 | Chemical fate modelling (Manuele Margni): Overview of typical environmental mass balance concepts; Introduction to transport and degradation rate calculations as well matrix solutions + short exercise (conduct a mass balance and calculate concentrations/rates on a 2-compartment system). |
| 09.45 - 10.30 | Human Exposure Modelling (Tom Mc Kone): Overview of human exposure concepts, including intake fraction, direct and indirect pathways, and subsistence vs. production-based approaches to food-based exposures + short exercise (calculate intake fractions for direct and indirect intake). |
| *10.30 - 10.50* | *Coffee break* |
| 10.50 - 11.30 | Human Exposure Modelling (continuation) |
| 11.30 - 12.30 | Human Effects Modelling (Olivier Jolliet): Overview of concepts and estimation techniques to determine risk-based and DALY-based effect factors and overall characterisation factors + short exercise (calculate effect factors for carcinogenic |

and non carcinogenic chemicals).

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| *12.30 - 13.45* | *Lunch* |
| 13.45 - 14.30 | <u>Ecotoxicological Effects Modelling</u> (Olivier Jolliet): Overview of concepts and estimation techniques using test data to determine effect factors and overall characterisation factors + short exercise (calculate ecotoxicological effect factors). |
| 14.30 - 14.50 | <u>Calculation of overall characterization factors</u> (Tom Mc Kone): combine fate, exposure and effect modelling steps into a unique metric. |
| *14.50 - 15.10* | *Coffee break* |
| 15.10 - 15.40 | <u>Review exercise with simplified matrices</u> (Ralph Rosenbaum) <br> <u>Source to impact framework and uncertainty</u> (Ralph Rosenbaum): presentation of the matrix approach, the USETox model and uncertainty assessment. <br> Illustrative examples on how to interpret modelling results. |
| 15.40 - 16.40 | <u>Overall Modelling</u> with software: Provision of straightforward examples from raw data sets to estimate and interpret characterisation factors for human health and ecotoxicological impacts <u>using the USEtox model</u> for organics (supervised by all instructors). |
| 16.40 - 17.00 | <u>Concluding remarks</u> (all instructors) |

**Products / course materials:**
* Short course handouts will be distributed
* A copy of the USEtox model will be distributed

**Participants to bring their own laptop to the course:**
Yes

**Instructors:**
Timothy Iannuzzi (ARCADIS, USA), David Ludwig (ARCADIS, USA)

**Course length:**
Full day (8.00-17.00 hrs)

**Course level:**
Introductory - Intermediate

**Description:**
This course will provide a broad introduction into the science and practice of Ecological Risk Assessment (ERA), and will utilize case study examples to generate participant-instructor discussion on the practice of weight-of-evidence ERA, as well as principles and issues of risk management. While the focus will be primarily on chemical contaminants, a broad array of multi-stressor issues will also be covered. This will be a good course for participants with little or no experience in ERA, as well as those with a moderate level of understanding of the practice.
The course will be broken down into two main modules (morning and afternoon sessions). The first module will cover a broad overview of the ERA process and frameworks, along with a concise introduction to several scientific principles and disciplines that are key to ERA practicioners. These include basic systems ecology, toxicology, population biology, fate and transport of chemicals in the environment, empirical and applied modeling, environmental data, and regulatory policy and guidelines. Materials will be provided to the course participants for suggested follow-up study in each of these technical area. These will include lists of suggested readings(including a focused list of SETAC publications on the subject matter) and internet sites, terminology/definition sheets, and a computer "thumb drive" that contains electronic versions of key ERA regulations, guidance documents, and related materials.
The second module will focus on application of the ERA process to current environmental issues around the world. Case studies will be used to frame discussion on the broad application of the ERA framework to environmental issues, and risk management decision-making. The overall goal of this module will be to demonstrate how the ERA process/framework can be used to think about and evaluate a broad array of environmental issues from localized contaminated sites to large-scale issues such as climate change.

**Objectives:**
(1) Provide an introduction to the Ecological Risk Assessment (ERA) process and frameworks.
(2) Provide a broad overview of key technical topics that are important to ERA practitioners.
(3) Generate discussion between the participants and instructors on case examples and issues related to ERA process and its application to present environmental issues.
(4) Provide handouts and resource lists for participants to continue learning about the key technical and regulatory topics that are covered in the course.

**Course outline:**
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| 08.00 - 10.00 | (1) | Introduction to Course/Concepts of Risk Assessment |
| | (2) | Ecological Risk Assessment Approaches/Applications |
| | (3) | Sources of risk in the environment: human/ecological |
| | (4) | Basic systems ecology principles |
| *10.00 - 10.15* | *Coffee break* | |
| 10.15 - 12.00 | (5) | Introduction to environmental chemistry & toxicology |
| | (6) | Ecological Risk Assessment Framework & Process |
| | (7) | Problem Formulation & Conceptual Models |
| | (8) | Exposure Assessment |
| *12.00 - 13.00* | *Lunch* | |
| 13.00 - 15.00 | (9) | Effects Assessment |
| | (10) | Risk Characterization/Weight-Of-Evidence |
| | (11) | Uncertainties Assessment |
| | (12) | Environmental data: types and needs |

*15.00 - 15.15    Coffee break*
15.15 - 17.00    (13) Analytical tools for ERA
                       (14) Risk Management
                       (15) Case Studies and ERA Process Application
                       (16) The future of ecological risk assessment

**Products / course materials:**
- MS Power Point presentation materials and handouts of selected regulatory and technical materials will be used to teach this course and generate topical discussions on current environmental issues where Ecological Risk Assessment is applicable as an assessment tool.
- Binders of all presentation materials will be presented to the course attendees that contain areas for taking notes.
- Computer "thumb drives" of the course materials, as well as key regulations and technical support materials will be given to each participant.

**Participants to bring their own laptop to the course:**
No