



# SETAC Europe 19<sup>th</sup> Annual Meeting

31 May – 4 June 2009, Göteborg, Sweden



## LIST OF SHORT COURSES

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## SHORT COURSE 1: ADVANCES IN LCI MODELLING

**Instructors:**

Paolo Masoni (ENEA, Italy), Reinout Heijungs (Institute of Environmental Sciences (CML), Department of Industrial Ecology, The Netherlands), Tomas Ekvall (IVL Swedish Environmental Research Institute, Sweden)

**Course length:**

Full day (08:15 - 17:15)

**Course location:**

Göteborg Convention Centre, Room J1

**Course level:**

Advanced

**Description:**

In the last years a vivid debate has been opened on several methodological issues, with special focus on LCI modelling. Several contributions have been proposed to deepen the current LCI modelling, by including more mechanisms (beyond technological relations) and sophistication, like: economic relations; inclusion of behavioural aspects; time and space modelling; etc. in order to improve reliability, significance and usability of LCA applications.

This short course is designed to provide participants with new insight on LCI modelling, with focus on the consequential modelling, as an approach that takes into account the consequences of the actions and their interrelations, projecting the problem at market level, with all its dynamics. In this context partial equilibrium modelling, experiences curves and rebound effects become relevant and they will be dealt with during the course.

As the robustness of methods applied have to be guaranteed in order to provide sound and scientific based information, special attention will be given to uncertainty analysis. The course will start out by current ISO-LCA, moving towards the analysis of the most promising approaches, and will give an overview of the new research lines and programmes in the field of life cycle analysis, as resulting by the CALCAS project ([www.calcasproject.net](http://www.calcasproject.net)).

**Objectives:**

The objectives of the course are the following:

- To provide an insight on the new topics and research line in the field of life cycle analysis, starting from the definition of a Scientific Framework for LCA.
- To provide participants with practical approaches for the analysis of micro-economic relations into life cycle analysis. Supply and demand mechanisms, including substitution mechanisms are relevant for sustainability decision support; the income elasticity of demand, behavioural mechanisms, etc. are currently lacking in LCA but first approaches are presented in literature, having as a common starting point the consequential approach. All these elements are clearly reflected in the modelling for decision support.
- To strengthen knowledge on uncertainty analysis in LCA at the level of parameter, model and scenario, at present often underestimated. Indeed, it should become routine practice, due to the influence of choices to final LCA results.
- To contribute to the fostering of life cycle analysis, as a fundamental and comprehensive approach for sustainability assessment, into academic curricula. Indeed the issues of the short course and the materials (scientific papers and other publications) could be used also by other students and teachers for training purpose in educational organisations.

**Outline:**

- 08:15 - 09:15      Theoretical background and research perspectives (Reinout Heijungs)  
Course material on the scientific framework of LCA: State of the art of ISO-LCA, with its limitations; definition of a scientific framework for a new LCA as improved life cycle based system analysis for sustainability governance; future research lines.
- 09:15 - 09:45      Introduction to the nature of modelling in LCI (Tomas Ekvall)  
Course material on the main modelling options: static and dynamic models, linear and non-linear models, simulation and optimisation, input/output and hybrid

	modelling, etc.
09:45 - 10:00	<i>Coffee Break</i>
10:00 - 10:30	Consequential approach (Tomas Ekvall) Course material on the consequential approach from qualitative to quantitative implementation: where we are, what is still missing, which approaches are available for taking into account the consequences of the actions at market level: partial equilibrium modelling, experience curves, rebound effects, etc.
10:30 - 11:00	Choosing between attributional and consequential LCA (Tomas Ekvall) Course material on the practical, theoretical, and moral pros and cons of the two approaches
11:00 - 12:00	Discussion on attributional and consequential LCA
12:00 - 13:00	<i>Lunch break</i>
13:00 - 14:45	Uncertainty management (instructor: Heijungs) Course material on the nature, sources, propagation and management of uncertainty in LCA.
14:45 - 15:00	<i>Coffee Break</i>
15:00 - 16:30	Uncertainty management, continued (instructor: Heijungs) Exercises on uncertainty and life cycle interpretation (please bring your own laptop running MS-Windows).
16:30 - 17:00	Discussion on uncertainty management
17:00 - 17:15	Course evaluation

### **Products / course materials:**

The course will use lectures, handouts, and web-based materials. Two weeks before the starting of the short course, instructors will provide participants with materials (scientific papers and other publications) on the topics of the course, in order to align the background of participants. A training version of CMLCA software, developed by CML, will be made available on CD and it will be used for exercises on uncertainty.

Participants will be provided also with the documentation produced within CALCAS project, in particular:

- A scientific framework for LCA: The document proposes a framework for New LCA, an improved life cycle based system analysis for sustainability governance, by revising the ISO-framework for LCA and defines the main elements in terms of structure and mechanisms/relations considered.
- Critical review of ISO-LCA: The document presents a review of the scientific literature on ISO-LCA, in order to identify intrinsic limits of ISO-LCA and elements for the deepening and broadening of the methodology.

CALCAS is an EU 6th Framework Co-ordination Action for innovation in Life-Cycle Analysis for Sustainability, aiming to achieve this efficacy increase. CALCAS will go beyond the boundaries of ISO-LCA. Going beyond ISO-LCA, might be called Life Cycle Analysis approaches, as is done in the 4th call of FP6. However, both Life Cycle Assessment and Life Cycle Analysis are abbreviated to LCA. Therefore, within the CALCAS project we will refer to (new) LCA, a result of innovation, in contrast to ISO-LCA. The general objective of CALCAS is to develop ISO-LCA by:

- "deepening" the present models and tools to improve their applicability in different contexts while increasing their reliability and usability
- "broadening" the LCA scope by better incorporating sustainability aspects and linking to neighboring models, to improve their significance
- "leaping forward" by a revision/enrichment of foundations, through the crossing with other disciplines for sustainability evaluation.

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

Yes

## SHORT COURSE 2a: FROM UNSEQUENCED SPECIES TO ANALYZED GENE EXPRESSION MICROARRAY – THEORY ONLY

**Instructors:**

Noomi Asker (University of Gothenburg, Sweden), Erik Kristiansson (University of Gothenburg, Sweden)

**Course length:**

Half day (THEORY ONLY) (08:00 - 12:00)

**Course location:**

Göteborg Convention Centre, Room R21

**Course level:**

Introductory

**Description:**

The objective of the course is to understand the needs, possibilities and limitations for setting up a large-scale gene expression project starting with a non-sequenced species. The DNA microarrays, which are the standard techniques for these kinds of assays, are important tools for understanding the low-level molecular effects cause by exposures of toxicants. However, microarray-based gene expression measurements require a substantial amount of sequence information from the target species. In this course you will learn how low cost high-throughput sequencing can be used to generate sufficient information of a transcriptome for assembly of interesting genes. Furthermore, we show how this data can be used to design oligonucleotide microarrays for gene expression assays. You will understand i) the basics in modern high-throughput sequencing and how to process and analyze the sequence data, ii) how to design and perform a gene expression microarray experiment and iii) how to statistically interpret the resulting microarray data.

**Objectives:**

The objective of the course is to understand the needs, possibilities and limitations for setting up a large-scale gene expression project for a non-sequenced species.

**Outline:**

08:00 – 08:30	Introduction Scope and aim of the course (Noomi Asker)
08:30 – 09:00	Massively parallel pyrosequencing Introduction to high-throughput sequencing using 454 technology (Noomi Asker)
09:00 – 09:30	Transcriptome characterization using massively parallel pyrosequencing De novo transcriptome sequencing, assembly of transcripts, annotation (Erik Kristiansson)
09:30 – 10:00	<i>Coffee Break</i>
10:00 – 10:30	Transcriptome characterization using massively parallel pyrosequencing Example: The sequencing of the transcriptome of <i>Zoarces viviparus</i> . (Erik Kristiansson)
10:30 – 11:15	Gene expression profiling using microarrays Introduction to gene expression microarrays. Microarray analysis using the Geniom platform. (Noomi Asker)
11:15 – 11:45	Microarray design and analysis of microarray data Introduction to microarray design and analysis. Standard algorithms and procedures. (Erik Kristiansson)
11:45 – 12:00	Questions

**Products / course materials:**

The course material will be distributed to the participants as handouts.

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

No

## SHORT COURSE 2: FROM UNSEQUENCED SPECIES TO ANALYZED GENE EXPRESSION MICROARRAY – THEORY AND PRACTICE

### Instructors:

Noomi Asker (University of Gothenburg, Sweden), Erik Kristiansson (University of Gothenburg, Sweden), Ioannis Amarantos (Febit Biomed gmbh, Germany)

### Course length:

Full day (THEORY AND PRACTICE) (08:00 - 17:30)

### Course location:

Morning session (08:00 - 12:00) at the Göteborg Convention Centre, Room R21, afternoon session (13:30 - 17:30) at the Zoological department of Göteborg University

### Course level:

Introductory

### Description:

The objective of the course is to understand the needs, possibilities and limitations for setting up a large-scale gene expression project starting with a non-sequenced species. The DNA microarrays, which are the standard techniques for these kinds of assays, are important tools for understanding the low-level molecular effects cause by exposures of toxicants. However, microarray-based gene expression measurements require a substantial amount of sequence information from the target species. In this course you will learn how low cost high-throughput sequencing can be used to generate sufficient information of a transcriptome for assembly of interesting genes. Furthermore, we show how this data can be used to design oligonucleotide microarrays for gene expression assays. You will understand i) the basics in modern high-throughput sequencing and how to process and analyze the sequence data, ii) how to design and perform a gene expression microarray experiment and iii) how to statistically interpret the resulting microarray data. A practical part will be offered in the afternoon. This will include running a microarray experiment, involving hybridization, washing and detection of a DNA microarray chip.

### Objectives:

The objective of the course is to understand the needs, possibilities and limitations for setting up a large-scale gene expression project for a non-sequenced species.

### Outline:

08:00 – 08:30	Introduction Scope and aim of the course (Noomi Asker)
08:30 – 09:00	Massively parallel pyrosequencing Introduction to high-throughput sequencing using 454 technology (Noomi Asker)
09:00 – 09:30	Transcriptome characterization using massively parallel pyrosequencing De novo transcriptome sequencing, assembly of transcripts, annotation (Erik Kristiansson)
09:30 – 10:00	<i>Coffee Break</i>
10:00 – 10:30	Transcriptome characterization using massively parallel pyrosequencing Example: The sequencing of the transcriptome of <i>Zoarces viviparus</i> . (Erik Kristiansson)
10:30 – 11:15	Gene expression profiling using microarrays Introduction to gene expression microarrays. Microarray analysis using the Geniom platform. (Noomi Asker)
11:15 – 11:45	Microarray design and analysis of microarray data Introduction to microarray design and analysis. Standard algorithms and procedures. (Erik Kristiansson)
11:45 – 12:00	Questions
12:00 – 13:30	<i>Lunch break</i>

13:30 – 14:15	Introduction to the Geniom platform (Ioannis Amarantos)
14:15 – 15:15	Running a microarray experiment: Injection and hybridization (Ioannis Amarantos)
15:15 – 15:30	<i>Coffee Break</i>
15:30 – 17:15	Running a microarray experiment: Washing and detection (Ioannis Amarantos)
17:15 – 17:30	Course evaluation

**Products / course materials:**

The course material will be distributed to the participants as handouts.

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

No

## SHORT COURSE 3: HOW TO BEST CONDUCT AND REPORT AQUATIC ECOTOXICITY TESTS ACCORDING TO THE INTERNATIONAL GUIDELINES

**Instructors:**

Hans Rufli (ecotoxsolutions, Switzerland)

**Course length:**

Full day (08:00 - 17:00)

**Course location:**

Göteborg Convention Centre, Room R22

**Course level:**

Intermediate

**Targeted 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 GEeD 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. Thus, it provides the knowledge and skills to optimise the testing in order to avoid the production of invalid data and the repetition of tests.

Guidance will be given on how to best interpret and express study results in a scientifically meaningful way. A case study based on an acute fish test with a 'difficult to test substance' will illustrate reporting needs and deficiencies. Practical examples will be discussed on how to best report results of aquatic ecotoxicology studies.

Last but not least, the course will provide information on the philosophy of testing and its background beyond what is stated in the guidelines, on effect -concentration and timeconcentration relationships, on extrapolations from results of acute to chronic tests and from laboratory test results to effects in the environment.

**Objectives:**

At the end of the course, each participant should know:

- how to perform tests in order to meet the requirements of several regulatory authorities and what makes a study to "not satisfy guideline requirements" for the authorities;
- how to report and express the results of ecotoxicology studies in a consistent, clearly represented and scientifically meaningful way;
- how are effects related to concentration and time as well as to different life stages;
- how are acute related to chronic test results and laboratory test results to the environment.

**Outline:**

- Test requirements for algae-, daphnia- and fish tests according to the various guidelines, and recommendations on how to perform tests in order to generate valid data acceptable to the regulatory authorities as exemplified by reactions of the authorities to specific studies.
- Guidance on reporting ecotoxicological studies, particularly on a scientifically consistent and meaningful expression of toxicity data discussed using practical examples.
- Background information on the philosophy of toxicity testing, concentration-effect and concentration-time relationships, and relations between results of laboratory tests and effects in the environment.

8:00 - 8:30            General Introduction: Introduction of participants, illustration of objectives, distribution of handouts

8:30 - 9:15            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.

9:15 - 9:45	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
9:45 - 10:00	<i>Coffee break</i>
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	<i>Lunch</i>
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	<i>Coffee break</i>
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:**

File containing handouts (A4-format) of the presentations and summaries for future use.

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

No

## SHORT COURSE 5: MICROARRAY TECHNOLOGY – FROM EXPERIMENTAL DESIGN TO APPLICATIONS

**Instructors:**

Dries Knapen (University of Antwerp, Belgium), Wim De Coen (ECHA, Finland)

**Course length:**

Full day (09:45 - 17:30)

**Course location:**

Göteborg Convention Centre, Room R23

**Course level:**

Intermediate

**Description:**

Microarray technology plays an increasingly important role in contemporary research. However, there is a growing discrepancy between theoretical (mathematical) considerations when analysing microarray data, and the approach taken by life scientists. Numerous articles in bioinformatics and biostatistics-oriented journals suggest best practices and propose new algorithms for use in gene expression studies. Unfortunately, it appears that this information does not sufficiently reach scientists using microarray technology in their research. Furthermore, it appears to be a non-trivial task to translate the results of a typical gene expression experiment into a biologically meaningful hypothesis, and to link these results to effects that are observed at higher levels of biological organisation. Finally, the real-life value of transcriptomics data in risk assessment, categorisation of chemicals, and the potential of the implementation thereof in legislation is often not well understood. Therefore, this short course will provide an overview of the most important milestones in a study using microarray technology: from designing microarray experiments, analysing the raw data, interpreting the resulting lists of differentially expressed genes, to a primer of the potential of transcriptomics data in the REACH legislation. By outlining the complete workflow, this course will help scientists to better design and interpret future microarray experiments.

**Objectives:**

1. Learn to design statistically powerful microarray experiments;
2. Review the basic raw data analysis steps through a R/Bioconductor demonstration;
3. Review techniques to make sense of lists of differentially expressed genes to answer specific, biologically relevant questions;
4. Help focusing future genomics research by providing an overview of how gene expression data can/will be used in legislation (REACH).

**Outline:**

09:45 - 10:00	<i>Coffee</i>
10:00 - 11:00	Introduction to microarray technology (Dries Knapen and Wim De Coen; co-presenting: An Hagensnaars)
11:00 - 12:00	Experimental and hybridization design of microarray experiments (Dries Knapen)
12:00 - 13:00	<i>Lunch break</i>
13:00 - 13:30	Discussion of topics covered in the morning session (Dries Knapen and Wim De Coen)
13:30 - 14:45	Microarray data analysis using R and Bioconductor: demo (Dries Knapen; co-presenting: Lucia Vergauwen)
14:45 - 15:00	<i>Coffee Break</i>
15:00 - 15:45	The next step: making sense of differentially expressed gene lists (Dries Knapen; co-presenting: Nathalie Dom)
15:45 - 17:00	Application of microarray data in a regulatory context: REACH and genomics (Wim De Coen)
17:00 - 17:30	Discussion and questions (Dries Knapen and Wim De Coen)

**Products / course materials:**

- Printed copy of presented slides, in the form of a book.
- USB flash drive containing digital copies of the slides, and additional resources such as open-source data analysis packages, urls to relevant webpages, ...

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

No

## SHORT COURSE 6: MODELLING COMPARATIVE RISK OF TOXICS ON HUMANS AND ECOSYSTEMS

**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 (08:00 - 17:00)

**Course location:**

Göteborg Convention Centre, Room R24

**Course level:**

Intermediate

**Targeted 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 were 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.

**Outline:**

08:00 - 08:15	Welcome
08:15 - 08:30	General introduction: source to damage cause-effect chain relationship and modelling steps (M. Margni)
08:30 - 09:45	Chemical fate modelling: 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 (M. Margni)
09:45 - 10:30	Human Exposure Modelling: 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 (T.

	McKone)
10:30 – 10:50	<i>Coffee Break</i>
10:50 – 11:30	Human Exposure Modelling (continuation)
11:30 – 12:30	Human Effects Modelling: 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 (O. Jolliet)
12:30 – 13:45	<i>Lunch</i>
13:45 – 14:30	Ecotoxicological Effects Modelling: Overview of concepts and estimation techniques using test data to determine effect factors and overall characterisation factors Short exercise: calculate ecotoxicological effect factors (O. Jolliet)
14:30 - 14:50	Calculation of overall characterization factors: combine fate, exposure and effect modelling steps into a unique metric (O. Jolliet)
14:50 - 15:10	<i>Coffee Break</i>
15:10 – 15:40	Source to impact framework and uncertainty: presentation of the matrix approach, the USETox model and uncertainty assessment. Illustrative examples on how to interpret modelling results (R. Rosenbaum)
15:40 – 16:40	Overall Modelling with software: Provision of straightforward examples from raw data sets to estimate characterisation factors for human health and ecotoxicological impacts using the USEtox model for organics (supervised by all instructors)
16:40 – 17:00	Concluding remarks (all instructors)

**Products / course materials:**

Short course handouts and a copy of the USEtox model will be distributed.

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

Yes

## SHORT COURSE 7: NANOTECHNOLOGY AND THE ENVIRONMENT

### Instructors:

Kathleen Sellers (Arcadis, USA), co-instructors to be determined

### Course length:

Half day (13:00 - 17:00)

### Course location:

Göteborg Convention Centre, Room R21

### Description:

One estimate suggests that nanotechnology could grow to \$3.1 trillion of the global manufacturing economy by 2016. Nanotechnology is revolutionizing the manufacture of many products, including clothing, paints and coatings, medicines and diagnostic systems, cosmetics, electronics, and even food. Some have described doomsday scenarios of the environmental consequences, and public surveys have shown that the public distrusts the ability of the government or corporations to manage nanotechnology wisely. Yet new nanotechnology-based products enter the market frequently, with some 800 consumer products now on the market.

This course will discuss the "nanotechnology revolution" and its environmental implications, including the following topics:

- Terminology, basic principles, and manufacturing processes
- Applications
- Environmental concerns
  - Critical properties
  - Fate and transport in the environment
  - Potential exposures
  - Effects of exposure
- Regulatory protections
- Life Cycle thinking

Important points will be illustrated with case studies.

The course will be updated from the short course "Nanotechnology and the Environment" which was presented at the SETAC North America 29th Annual Meeting in November 2008. It is based in part on the book "Nanotechnology and the Environment" (CRC Press, 2008), which Ms. Sellers edited and co-wrote.

### Objectives:

The objective of this course is to provide attendees with a working knowledge of the behaviour of nanomaterials in the environment, potential exposures and resulting risks, and the challenges posed in developing science and regulations.

### Outline:

13:00 - 13:20	Nanotechnology primer <ul style="list-style-type: none"><li>a. Terminology</li><li>b. Basic principles</li><li>c. Manufacturing processes</li><li>d. Applications</li></ul>
13:20 - 14:00	Exposure <ul style="list-style-type: none"><li>a. Life cycle considerations</li><li>b. Fate and transport processes</li><li>c. Mass balance</li><li>d. Case study: nano silver</li></ul>
14:00 - 14:45	Potential risks <ul style="list-style-type: none"><li>a. Determinants of toxicity</li><li>b. Potential effects (by exposure route)</li><li>c. Risk communication</li></ul>
14:45 - 15:00	<i>Coffee Break</i>
15:00 - 15:30	<ul style="list-style-type: none"><li>d. Case study: carbon nanotubes</li><li>e. Case study: nano titanium dioxide</li></ul>

- 15:30 - 16:00 Regulatory developments  
a. European Union  
b. United States
- 16:00 - 16:30 Life Cycle thinking  
a. Frameworks and limitations  
b. Case study: Carbon nanotubes  
c. Case study: nano zero valent iron
- 16:30 - 17:00 Review, questions, and course evaluation

**Products / course materials:**

Handouts of presentation.

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

Not needed but helpful

## SHORT COURSE 8: PETROTOX – A TOOL FOR THE HAZARD ASSESSMENT OF PETROLEUM SUBSTANCES

**Instructors:**

Aaron Redman (HydroQual, USA), Thomas Parkerton (ExxonMobil Biomedical Sciences), Stuart Forbes (Shell)

**Course length:**

Half day (08:00 - 12:00)

**Course location:**

Göteborg Convention Centre, Room R25

**Course level:**

Introductory

**Targeted audience:**

Mostly graduate students

**Description:**

Petroleum substances (e.g. gasoline, kerosene, etc.) are complex substances derived from crude oils. These are of undefined and variable composition, consisting of hundreds to thousands of individual hydrocarbons. This complexity presents challenges for environmental hazard assessment. The hydrocarbon block method was developed in the EU for practically assessing the hazards and risks of these complex substances.

This course will cover the subject areas relevant to the implementation of the hydrocarbon block methods (HBM) for the hazard assessment of petroleum substances. Experimental methods that are used to generate aquatic toxicity hazard data for petroleum substances will be discussed. Analytical methods used to characterize the composition of petroleum substances will be reviewed. The remainder of the course will describe a user-friendly, publicly available spreadsheet model (PETROTOX) that predicts aquatic or wastewater organism toxicity of complex petroleum substances. PETROTOX couples a multi-component partitioning sub-model with the target lipid model to evaluate effects. The model also has the capability to model HC5 values for individual hydrocarbons and hydrocarbon blocks, so can directly support the risk assessment of petroleum products.

The principles used in the development and calibration of PETROTOX will be presented. Validation of this tool, as well as potential applications, will be described.

**Objectives:**

Present and discuss the technical basis of the experimental methods and models used to assess environmental hazards of complex petroleum substances. Participants will learn recent analytical, ecotoxicological and modelling methods used to assess this commercially important group of substances.

**Outline:**

08:00 – 08:15 Introduction to petroleum products (T. Parkerton)

- manufacture
- composition & properties
- product categories

08:15 – 09:00 Analytical Methods for Petroleum Product Characterization (S. Forbes)

- conventional methods/composition vs. boiling point
- improved methods/composition vs. boiling point and hydrocarbon class
  - TPH working group method (low-resolution)
  - 2d-gc method (high resolution)

- 09:00 – 09:30 Aquatic Toxicity Assessment (T. Parkerton)
- Assessment of individual chemicals
  - WAF test procedure
  - Other test methods
  - Predictive methods / overview of PETROTOX
    - WAF Exposure Model
    - Target Lipid Effect Model
- 09:30 – 09:45 WAF Exposure Model (A. Redman)
- Review of Raoult's & Henry's Law
  - Predicting multi-component dissolution of simple hydrocarbon mixture
    - no headspace
    - with headspace
  - Predicting multi-component dissolution of a complex hydrocarbon mixture in a WAF test system
- 09:45 – 10:00 *Coffee break*
- 10:00 – 10:30 Target Lipid Effects Model (A. Redman)
- CBR concept & derivation of TLM framework
  - Calibration to acute toxicity datasets
  - Extension to chronic toxicity prediction using ACRs
  - Toxicity cut-offs and extension to high Log Kow hydrocarbons
  - PNEC derivation using TLM species sensitivity distributions
- 10:30 – 11:00 PETROTOX Description (A. Redman)
- User Inputs
  - Representative structure-property library
  - Mapping product composition to the library
  - Hydrocarbon Additivity and Toxic Units
  - Model Outputs
  - Model Assumptions
  - Preliminary validation
  - Applications / Future Uses
- 11:00 – 11:30 PETROTOX Demonstration (Course Instructors)
- 11:30 – 12:00 Review, questions and course evaluation

**Products / course materials:**

Re-prints of relevant published articles, handouts of lecture slides, CD with presentations and other course materials including a demonstration version of the PETROTOX spreadsheet model.

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

Yes

## SHORT COURSE 9: PHYSICOCHEMICAL CHARACTERIZATION OF NANOMATERIALS

### Instructors:

Martin Hassellöv (University of Gothenburg, Sweden), Frank von der Kammer (University of Vienna, Austria), Julian Gallego (University of Gothenburg, Sweden), Perez Holmberg (University of Gothenburg, Sweden)

### Course length:

Full day (08:00 - 17:30)

### Course location:

Göteborg University - Chemistry Department (directions can be downloaded at [http://goteborg.setac.eu/embed/downloads/Map\\_to\\_short\\_course\\_9.pdf](http://goteborg.setac.eu/embed/downloads/Map_to_short_course_9.pdf))

### Course level:

Introductory-intermediate

### Description:

Adverse effects of nanomaterial have been shown for many ecotoxicological studies, but the results are not always comparable and sometimes even contradictory, much due to a lack of control of dispersion protocols and of physico-chemical characterization. Here we will provide ecotoxicologists and environmental chemists an opportunity to learn more on theory and get hands-on experience with a set of important, complementary characterization techniques.

### Objectives:

To study the environmental impact of nanomaterials it is essential to know the fundamental processes that regulate fate and behaviour as well as uptake and toxicity. Since these are very different for nanoparticles and conventional chemicals, it is crucial to determine these governing processes.

The course objective is to train ecotoxicologists and environmental chemist some fundamentals of colloidal nanomaterial dispersions (dispersive and aggregative forces, aggregation processes, stabilization) and more importantly how to characterize the most important physicochemical properties (size distributions, surface charge, zeta potential, morphology of agglomerates, composition etc).

### Outline:

8:00 - 8:15	Introduction and practical information (Martin Hassellöv)
8:15 - 9:00	Theory: Nanoparticle properties, dispersion and agglomeration (Frank von der Kammer)
9:00 - 9:45	Theory: Overview of characterization methods & analytical considerations (Martin Hassellöv)
9:45 - 10:00	<i>Coffee Break</i>
10:00 - 12:00	Hands on session 1
12:00 - 12:45	<i>Lunch break</i>
12:45 - 14:45	Hands on session 2
14:45 - 15:00	<i>Coffee Break</i>
15:00 - 17:00	Hands on session 3
17:00 - 17:15	Discussions & questions
17:15 - 17:30	Course evaluation

The hands-on sessions include about 15 min method-specific theory and 1:45 min experiments.

	Dynamic Light Scattering & Laser Doppler velocimetry (z-potential) (Perez Holmberg, Frank von der Kammer)	Nanoparticle Tracking Analysis (Julian Gallego)	Field-Flow Fractionation (Martin Hassellöv, Frank von der Kammer)
Hands-on session 1 (10:00 - 12:00)	Group 1	Group 3	Group 2
Hands-on session 2 (12:45 - 14:45)	Group 2	Group 1	Group 3
Hands-on session 3 (15:00 - 17:00)	Group 3	Group 2	Group 1

**Products / course materials:**

Hassellöv, M., Readman, J., Ranville, J. and Tiede, K. Nanoparticle analysis and characterization methodology in environmental risk assessment of engineered nanoparticles. *Ecotoxicology* 2008. Vol. 17, p. 344–361.

## SHORT COURSE 10: STATISTICAL METHODS IN ECOTOXICOLOGY USING R

**Instructors:**

Christian Ritz (University of Copenhagen, Denmark), Christian B. Phipper (COPSAC (Copenhagen Studies On Asthma in Childhood), Denmark), Jens C. Streibig (University of Copenhagen, Denmark)

**Course length:**

Full day (08:00 - 17:30)

**Course location:**

Göteborg Convention Centre, Room R6

**Course level:**

Advanced

**Targeted 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 statistical and visualisation techniques are available in R. Therefore, it is an extremely powerful, free, and all-in-one alternative software to specialised commercial data analysis software currently used by many ecotoxicologists.

The course will focus almost entirely on giving the participants hands-on experience and a feel for the software. The course material will consist of a wide range of case-studies that, based on real toxicological data, will introduce ANOVA methods, linear, non-linear regression (including dose-response analysis), and logistic and Poisson regression models. There will also be case-studies on more advanced topics such as 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. 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 (statistics and visualization in one);
3. Provide hands-on experience for common types of data analysis (cookbook);
4. Enable participants to use the software on own problems (take-home software).

**Outline:**

08:00 - 08:15	Introduction/Welcome
08:15 - 09:45	Lecture: Introduction to R in the context of ecotoxicology (Presenter: Christian Ritz. The lecture will give a brief history of the development of R over the last decade. Moreover, basic functionality for data manipulation and visualization will be demonstrated. Essential details and issues in using R in different environments will be highlighted.)
09:45 - 10:00	<i>Coffee break</i>
10:00 - 12:00	Installation of R and hands-on case studies (Presenter: Christian B. Phipper and Jens C. Streibig. A step-by-step approach is taken to introduce the participants to the software programme. A few simple case studies are taken in plenum to ensure that initial obstacles are resolved.)
12:00 - 13:00	<i>Lunch break</i>
13:00 - 14:45	Case studies continued (Instructors: Christian B. Phipper, Christian Ritz, and Jens C. Streibig. Intensive assistance and guidance are offered to the participants. There are typically many questions as the participants struggle to understand how to use the software, how to write correct commands and how to interpret the output.)
14:45 - 15:00	<i>Coffee break</i>

- 15:00 - 17:00 Case studies continued ( or analysis of participants' own data)  
(Instructors: Christian B. Pipper, Christian Ritz, and Jens C. Streibig. Intensive individual assistance and guidance are offered to the participants. However, at this stage participants start to work on their on data and problems and therefore a wide range of statistical methods available in R are being applied, and therefore the instructors will provide individual advice in order to resolve specific statistical problems.)
- 17:00 - 17:15 Course evaluation
- 17:15 - 17:30 Conclusion

**Products / course materials:**

Hand-outs of the lecture note 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