Workshop Programme

Estimating toxicity thresholds for aquatic ecological communities from sensitivity distributions

11-13 February 2014, Amsterdam

Organised by

ecetoc And Environment Agency

ORGANISING COMMITTEE

Scott Belanger	Procter & Gamble
Peter Craig	University of Durham
Scott Dyer	Procter & Gamble
Malyka Galay Burgos	ECETOC
Mick Hamer	Syngenta
Andy Hart	FERA
Stuart Marshall	Unilever
Paul Whitehouse	Environment Agency

CONTENTS

INTRODUCTION

AIM

The workshop will discuss and report current thinking on when and how species sensitivity distributions, SSDs, should be used and how the methodology might be further developed. The workshop will consider three key aspects:

1) What is the ecological relevance of an SSD?

- Are we making ecologically relevant assessments? Are regulatory protection goals explicit and clear? Are they set in relation to environmental quality? How do prospective and retrospective approaches differ?
- Are all species of equal importance, or are there keystone species that are more important than others? If so, how might these be accounted for?
- Is a generic PNEC derived from an SSD overly simplistic in terms of ecological representativeness? Should we develop representative assemblages/communities (archetypes) to represent different typologies? Should protection goals account for local community composition?
- How does aquatic community sensitivity vary with species composition? (summary of and developments since Pellston Classic workshop 2001- Ecological Variability: Separating Natural from Anthropogenic Causes of Ecosystem impairment)
- How can knowledge of chemical MoA help construct SSDs for HC5 estimation?

2) What SSD statistical models are available for deriving toxic thresholds (HC5/PNEC) for aquatic communities?

- Review current tools and key (statistical) methodology, including assumptions about distributions of sensitivity, use of hierarchical models, interspecies correlations. Identify where there are important differences and what the implications of these could be.
- As sensitivity to chemical stress seems to be related to taxonomic closeness, how could this be used in the construction and interpretation of SSDs?
- Do models that utilise prior knowledge, e.g. aquatic toxicity data sets on many species, provide advantages over other methods?
- Are current modelling success criteria, such as those identified in the REACH TGD, sufficient, overly prescriptive or insufficient?

3) Regulatory application

- Would the methods reviewed in this workshop be accepted for use in regulatory assessments under current guidance? If not, what steps would be needed to facilitate their acceptance in the future?
- Should current guidance on the use of SSDs be revised in the light of the issues and approaches discussed in this workshop?
- What implications are there for the interpretation of SSDs and HC5s in risk assessment and risk management?

PROGRAMME DAY 1: TUESDAY 11 FEBRUARY

08:00 - 09.00	*Registration and coffee*	
09:00 - 09.10	**Welcome and introductory remarks**	**Organising Committee**
09:10 - 09.40	**Sense, simplicity and successes of SSDs in environmental protection, assessment and management**	**Leo Posthuma** RIVM, The Netherlands

What is the ecological relevance of an SSD?

Chair: Scott Belanger
P&G, USA

09:40 - 10:10	**Ecological limitations of SSDs**	**Lorraine Maltby** University of Sheffield, UK
10:10 - 10:40	**How do species traits influence sensitivity and herewith species sensitivity distributions?**	**Paul van den Brink** Alterra, The Netherlands
10:40 - 11:00	*Coffee break*	
11:00 - 11:30	**Field validation of species sensitivity distributions**	**Adam Peters** WCA Environment, UK
11:30 - 12:00	**Derivation of toxicity thresholds for LAS – integration of QSARs, SSDs, mesocosms, and field data**	**Scott Belanger** P&G, USA
12:00 – 12:30	**Field-based species sensitivity distribution and community sensitivity distribution as alternative ways for field validation of the PNECs derived from laboratory based approaches**	**Kenneth Leung** University of Hong Kong
12:30 - 13:30	*Lunch*	

13:30 - 15:00	**SYNDICATE SESSION 1: ECOLOGICAL CONSIDERATIONS**				
					Chair: Scott Belanger P&G, USA
Group:	**1A**	**1B**	**1C**	**1D**	
Moderator:	*L Maltby*	*L Posthuma*	*S Duquesne*	*K Solomon*	
Rapporteur:	*M Hamer*	*P Whitehouse*	*S Dyer*	*S Marshall*	

- Are we making ecologically relevant assessments? Are regulatory protection goals explicit and clear? Are they set in relation to environmental quality? How do prospective and retrospective approaches differ?
- Are all species of equal importance, or are there keystone species that are more important than others?
- Is a generic PNEC derived from an SSD overly simplistic in terms of ecological representativeness or should we develop representative assemblages/communities (archetypes) to represent different typologies? Should protection goals account for local community composition?
- How does aquatic community sensitivity vary with species composition?
- How can knowledge of chemical MoA help construct SSDs for HC5 estimation?
- What are the research needs?

15:00 - 16:00 **Plenary feedback & discussion with panel**

Chair: Scott Belanger and Mick Hamer

Breakouts report back (5-10 minutes each)
Identify key points, consensus and research needs

16:00 - 16:30 *Coffee break*

What SSD statistical models are available for deriving toxic thresholds (HC5/PNEC) for aquatic communities?

Chair: Peter Craig

16:30 - 16:50	**HC5 estimation in SSDs revisited**	**Tom Aldenberg** RIVM, The Netherlands
16:50 - 17:10	**Assessment factors for deriving PNECs: food for thought**	**Ad Ragas** Radboud University, The Netherlands
17:10 - 17:30	**Weight of evidence approaches for deriving HC5s**	**Sandrine Andres** INERIS, France
17:30 – 17:50	**Sample size in PNEC derivation**	**Scott Dyer** P&G, USA
17:50 – 18:10	**How to extrapolate across 100,000+ substances, sites and species with SSDs?**	**Jan Hendriks** Radboud University, The Netherlands

Close of first day

19:30 *Dinner*

PROGRAMME DAY 2: WEDNESDAY 12 FEBRUARY

What SSD statistical models are available for deriving toxic thresholds (HC5/PNEC) for aquatic communities?

Chair: Andy Hart
FERA, UK

09:00 - 09:30 **Interspecies correlation estimation (ICE) models predict supplemental toxicity data for SSDs**
Sandy Raimondo
US EPA, USA

09:30 - 10:00 **HC5s from taxonomically structured hierarchical species sensitivity distributions**
Peter Craig
University of Durham, UK

10:00 - 10.30 *Coffee break*

10:30 - 12:00 **Demonstration of the web-based interspecies correlation estimation (web-ICE) modelling application**
Peter Craig/ Mace Baron/Sandy Raimondo

12:00 - 13:00 *Lunch*

13:00 - 14:00 **Case studies Session**
Stuart Marshall, Mick Hamer, Scott Belanger and Peter Craig

Two case studies will be described and discussed using a surfactant LAS and a pesticide, chlorpyrifos. For each chemical, HC5s will be derived with available data using a range of SSD methods/tools. Different ecological scenarios will be assessed: stream, pond, marine.

14:00 - 15:00 **SYNDICATE SESSION 2: STATISTICAL CONSIDERATIONS**

Chair: Andy Hart
FERA, UK

Group:	**2A**	**2B**	**2C**	**2D**
Moderator:	*K Leung*	*R Wenning*	*A Ragas*	*P Chapman*
Rapporteur:	*P Craig*	*JP Gosling*	*M Barron*	*S Raimondo*

- Review current tools and key (statistical) methodology, including assumptions about distributions of sensitivity, use of hierarchical models, interspecies correlations. Identify where there are important differences and what the implications of these could be.
- As sensitivity to chemical stress seems to be related to taxonomic closeness, how could this be used in the construction and interpretation of SSDs?
- Do models based on prior knowledge provide advantages over other methods?
- What are the research needs?

15:30 - 16:00	*Coffee break*

16:00 - 17:00	**Plenary: feedback & discussion with panel**
	Chair: Andy Hart/Peter Craig
	Breakouts report back (5-10 minutes each)
	Identify key points, consensus and research needs

Regulatory Applications	
	Chair: Mace Barron US EPA, USA
17:00 - 17:30	**Regulatory application of SSDs in European regulations**
	Paul Whitehouse Environment Agency, England
17:30 – 18:00	**Regulatory use of SSDs in Australia and New Zealand**
	Michael Warne DSITIA Science Delivery, Australia

19:30	*Dinner*

Regulatory Applications

Chair: Paul Whitehouse
Environment Agency, England

08:30 - 09:00 **Use of SSD in China**
Fengchang Wu
Chinese Research Academy of Environmental Sciences

09:00 - 09:30 **Use of SSD to derive no-effect thresholds for water quality guidelines and ecological risk assessment in Canada**
Anne Gosselin
Environment Canada

09:30 - 10:00 **Use of SSDs in the USA – endangered species and water quality criteria**
Mace Barron
US EPA, USA

10:00 – 10:30 *Coffee break*

10:30 - 11:30 **SYNDICATE SESSION 3: REGULATORY CONSIDERATIONS**

Chair: Paul Whitehouse

Group:	**3A**	**3B**	**3C**	**3D**
Moderator:	A Peters	M Warne	A Gosselin	D de Zwart
Rapporteur:	M Hamer	S Belanger	M Barron	A Hart

- Would the methods reviewed in this workshop be accepted for use in regulatory assessments under current guidance? If not, what steps would be needed to facilitate their acceptance in the future? What are the opportunities to update technical guidance?
- Should current guidance on the use of SSDs be revised in the light of the issues and approaches discussed in this workshop, e.g. number of species?
- What implications are there for the interpretation of SSDs and HC5s in risk assessment and risk management?
- What are the research needs?

11:30 -12:30 **Plenary: feedback & discussion with panel**

Chair: Paul Whitehouse/Mace Barron

Breakouts report back (5-10 minutes each)
Identify key points, consensus and research needs

15:30 - 16:00	**Coffee break**	

12:30 - 13:30	**Final Plenary discussion: synthesis of key points and research needs from the three sessions** **Chair: Mick Hamer/Andy Hart/Paul Whitehouse** Identify key points and consensus What are the research needs? Next steps	

13:30 – 14:30	*Adjourn and lunch*

Close of Workshop

Suggested topics:

- Are we making ecologically relevant assessments? Are regulatory protection goals explicit and clear? Are they set in relation to environmental quality? How do prospective and retrospective approaches differ?
- Are all species of equal importance, or are there keystone species that are more important than others?
- Is a generic PNEC derived from an SSD overly simplistic in terms of ecological representativeness or should we develop representative assemblages/communities (archetypes) to represent different typologies? Should protection goals account for local community composition?
- How does aquatic community sensitivity vary with species composition?
- How can knowledge of chemical MoA help construct SSDs for HC5 estimation?
- What are the research needs?

Group 1A **Dam Room**

First Name	Name	Role
Lorraine	**Maltby**	Moderator
Mick	**Hamer**	*Rapporteur*
Tom	**Aldenberg**	
Timothy	**Barber**	
Peter	**Craig**	
Pepijn	**de Vries**	
Chenglian	**Feng**	
Guillaume	**Kon Kam King**	
Kenneth	**Leung**	
Adam	**Peters**	

Group 1B

Warmoes Room

First Name	Name	Role
Leo	**Posthuma**	Moderator
Paul	**Whitehouse**	*Rapporteur*
Scott	**Belanger**	
Christian	**Collin-Hansen**	
Charles	**Eadsforth**	
Malyka	**Galay Burgos**	
John Paul	**Gosling**	
Marion	**Junghans**	
Paul	**Van den Brink**	
Michael	**Warne**	
Richard	**Wenning**	

Group 1C

Executive Room

First Name	Name	Role
Sabine	**Duquesne**	Moderator
Scott	**Dyer**	*Rapporteur*
Mace	**Barron**	
Jean Lou	**Dorne**	
Anne	**Gosselin**	
Maike	**Habekost**	
Jan	**Hendriks**	
Christian	**Michel**	
Ad	**Ragas**	
Krishna Kumar	**Selvaraj**	
Fengchang	**Wu**	

Group 1D

Amsterdam Room

First Name	Name	Role
Keith	**Solomon**	Moderator
Stuart	**Marshall**	*Rapporteur*
Sandrine	**Andres**	
Peter	**Chapman**	
Dick	**de Zwart**	
Andy	**Hart**	
Ailbhe	**Macken**	
Yuan	**Pan**	
Sandy	**Raimondo**	
Hans	**Sanderson**	
Zhen-guang	**Yan**	

Suggested topics:

- Review current tools and key (statistical) methodology, including assumptions about distributions of sensitivity, use of hierarchical models, interspecies correlations. Identify where there are important differences and what the implications of these could be.
- As sensitivity to chemical stress seems to be related to taxonomic closeness, how could this be used in the construction and interpretation of SSDs?
- Do models based on prior knowledge provide advantages over other methods?
- What are the research needs?

Group 2A **Dam Room**

First Name	Name	Role
Kenneth	**Leung**	Moderator
Peter	**Craig**	*Rapporteur*
Tom	**Aldenberg**	
Timothy	**Barber**	
Pepijn	**de Vries**	
Chenglian	**Feng**	
Mick	**Hamer**	
Guillaume	**Kon Kam King**	
Lorraine	**Maltby**	
Adam	**Peters**	

Group 2B
Warmoes Room

First Name	Name	Role
Richard	**Wenning**	Moderator
John Paul	**Gosling**	*Rapporteur*
Christian	**Collin-Hansen**	
Scott	**Belanger**	
Charles	**Eadsforth**	
Malyka	**Galay Burgos**	
Marion	**Junghans**	
Leo	**Posthuma**	
Paul	**Van den Brink**	
Michael	**Warne**	
Paul	**Whitehouse**	

Group 2C
Executive Room

First Name	Name	Role
Ad	**Ragas**	Moderator
Mace	**Barron**	*Rapporteur*
Jean Lou	**Dorne**	
Sabine	**Duquesne**	
Scott	**Dyer**	
Anne	**Gosselin**	
Maike	**Habekost**	
Jan	**Hendriks**	
Christian	**Michel**	
Krishna Kumar	**Selvaraj**	
Fengchang	**Wu**	

Group 2D
Amsterdam Room

First Name	Name	Role
Peter	**Chapman**	Moderator
Sandy	**Raimondo**	*Rapporteur*
Sandrine	**Andres**	
Dick	**de Zwart**	
Andy	**Hart**	
Ailbhe	**Macken**	
Stuart	**Marshall**	
Yuan	**Pan**	
Hans	**Sanderson**	
Keith	**Solomon**	
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Suggested topics:

- Would the methods reviewed in this workshop be accepted for use in regulatory assessments under current guidance? If not, what steps would be needed to facilitate their acceptance in the future? What are the opportunities to update technical guidance?
- Should current guidance on the use of SSDs be revised in the light of the issues and approaches discussed in this workshop, e.g. number of species?
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Group 3A **Dam Room**

First Name	Name	Role
Adam	**Peters**	Moderator
Mick	**Hamer**	*Rapporteur*
Tom	**Aldenberg**	
Timothy	**Barber**	
Peter	**Craig**	
Pepijn	**de Vries**	
Chenglian	**Feng**	
Guillaume	**Kon Kam King**	
Kenneth	**Leung**	
Lorraine	**Maltby**	

Group 3B — Warmoes Room

First Name	Name	Role
Michael	**Warne**	Moderator
Scott	**Belanger**	*Rapporteur*
Christian	**Collin-Hansen**	
Charles	**Eadsforth**	
Malyka	**Galay Burgos**	
John Paul	**Gosling**	
Marion	**Junghans**	
Leo	**Posthuma**	
Paul	**Van den Brink**	
Richard	**Wenning**	
Paul	**Whitehouse**	

Group 3C — Executive Room

First Name	Name	Role
Anne	**Gosselin**	Moderator
Mace	**Barron**	*Rapporteur*
Jean Lou	**Dorne**	
Sabine	**Duquesne**	
Scott	**Dyer**	
Maike	**Habekost**	
Jan	**Hendriks**	
Christian	**Michel**	
Ad	**Ragas**	
Krishna Kumar	**Selvaraj**	
Fengchang	**Wu**	

Group 3D — Amsterdam Room

First Name	Name	Role
Dick	**De Zwart**	Moderator
Andy	**Hart**	*Rapporteur*
Sandrine	**Andres**	
Peter	**Chapman**	
Ailbhe	**Macken**	
Stuart	**Marshall**	
Yuan	**Pan**	
Sandy	**Raimondo**	
Hans	**Sanderson**	
Keith	**Solomon**	
Zhen-guang	**Yan**	

Sense, simplicity and successes of SSDs in environmental protection, assessment and management

Leo Posthuma
RIVM, the Netherlands

This contribution presents the versatile use of Species Sensitivity Distributions (SSDs) in environmental protection, assessment and management of environmental stress. There is sense, simplicity and success – despite shortcomings. Decades ago, the observation was made that sensitivities of different species towards a toxic compound are distributed such that it would fit a statistical model. This marked the birth of SSD-modeling. The concept helped to solve problems of that time. Soils and waters were affected by various compounds in the environment, and SSDs were used to set Environmental Quality Criteria. SSDs were one of the methods used to derive the so-called PNEC (Predicted No Effect Concentration) for ecosystems. Comparison of a PEC (Predicted Environmental Concentration) of a compound with its PNEC became a standard judgment method, applied to reduce toxic impacts in ecosystems, with PEC/PNEC-ratio's higher than unity signaling risk. Many concerns were (and are) voiced, a.o. on quality, number and relevance of input data of SSDs, model choice, and the PNEC itself. This workshop focuses, with today's knowledge, on SSD-issues – to support optimal decisions.

Since the invention of SSDs, holistic goals have been added to environmental policies. Water bodies should e.g. reach Good Ecological Status, next to Good Chemical Status. Furthermore, monitoring has revealed that exceedances of Criteria are frequent. These issues have triggered attention for applying SSDs in a second way: to derive local hazard levels from ambient exposures. In combination with mixture modeling, this use yields estimated values for the toxic pressure (of single chemicals or mixtures) of environmental samples. This use is currently frequent, in disciplines and approaches as variable as eco-epidemiological landscape-scale diagnosis of local impact causes, determining sanitation urgency in soil management, use in product Life Cycle Analysis, derivation of Chemical Footprints of current emissions, and impact reduction of chemical disasters around the globe by UN-field teams.

As yet, the dual use of SSDs has major practical implications in environmental protection and management, and that this expands beyond chemicals to stressors such as underwater noise, temperature and radionuclides, and beyond current techniques, such as via field-SSDs. Given the societal importance, the validity of SSD output is key. What does it mean when environmental concentrations increase? Does the predicted impact relate to observed impact? And if so, is it one-to-one, or at least linear? Confirmation study results suggest a nuanced outcome. SSD outputs clearly have sense, in that they rank impact degree, not kind – in a way helpful for the assessment goals. SSDs are simple, and they contain not a single bit of ecology, but they generate sensible outcomes for various problem definitions.

Past SSD applications have resulted in major environmental improvements (successes), which might best be envisaged by imagining the absence of concepts like the PNEC on the one hand, and the potentially affected fraction of species on the other. Reflections on the sense, simplicity and successes of SSDs provide the context within which potential improvements in the model can be designed.

Leo Posthuma

Leo Posthuma is currently research staff member of the Centre for Sustainability, Environment and Health at the Dutch National Institute for Public Health and the Environment, RIVM.

He is involved in the development, testing and validation of methods for ecological risk assessment and sustainable development. His research experience has included phytopathological studies and studies on the evolutionary ecology and population genetics of contaminant adaptation of exposed soil arthropod populations (PhD at VU Amsterdam). At RIVM he worked, amongst others, on community tolerance evolution, on bioavailability of toxic compounds, on joint effects of compound mixtures, on stability and resilience of soil ecosystems, on disaster management problems and on sustainability questions. He authored and co-authored many publications, acted as book editor and co-editor, and works on practicable tools for policy use, derived from the research. The book on SSDs which he co-edited and which was published in 2002 has collated the two formats of SSD use regarding theories and practices of that time.

ABSTRACT

Ecological limitations of SSDs

Lorraine Maltby
University of Sheffield, UK

Species sensitivity distributions are generally derived using data from single-species toxicity tests. The species used in these tests are often from a limited geographic and/or habitat range and toxicity is measured in the absence of interspecific interactions. SSDs are used to assess the risk of chemicals to ecological assemblages containing many interacting species, often in a range of habitats (e.g. rivers, ditches, ponds) in different geographic regions. This presentation will explore the potential ecological limitations of an SSD approach, with particular focus on pesticide risk assessment.

Lorraine Maltby

Lorraine Maltby is Professor of Environmental Biology at the University of Sheffield, UK and a NERC/Defra High Level Placement Fellow. Her fellowship is focussed on strengthening the uptake of science into policy and her research aims to understand how ecosystems respond and adapt to environmental stressors, including pollutants. She has over 100 peer-reviewed publications and has co-authored 3 books in ecotoxicology and risk assessment. Lorraine has served on UK government advisory committees and is past Chair of the Environment Panel of the Advisory Committee on Pesticides. She is currently a member of the Scientific Committee of the European Centre for Ecotoxicology and Toxicology of Chemicals and the UNEP Scientific Expert Group on Chemicals and the Environment. She was a member of the working group that produced the EFSA protection goals opinion.

How do species traits influence sensitivity and herewith species sensitivity distributions?

Paul J. van den Brink
Alterra and Wageningen University, the Netherlands

Species sensitivity distributions (SSD) assume that sensitivity to toxicants within target species is random. While the SSD approach has shown promise, it is limited by the fact that data are sparse for most compounds, and that these data are largely based on the lethal responses of a small group of testing lab species. Here I present an alternative approach, based on the hypothesis that organisms' sensitivity to stress is a function of their biology, and can be predicted from species traits such as morphology, life history, physiology and feeding ecology.

In this talk I will show a few examples on how species traits have been used to explain the differences in sensitivity between species.

I) Using data from the US EPA's AQUIRE database, we found that four species traits explained 71% of the variability in sensitivity to toxicants within a group of 12 species exposed to 15 chemicals. Our results indicate that this approach has promise, but effort is needed to compile species trait information to increase the power, precision and taxonomic representativeness of this approach.

II) Secondly, we mined existing data on organophosphate, carbamate and pyrethroid toxicity and mode of action and also species trait information. We linked taxon sensitivity to their traits at the family level in order to generate empirical and mechanistic hypotheses about sensitivity-trait relationships. In this way, we developed a Mode-Specific Sensitivity (MSS) ranking method, and tested this at the taxonomic level of family and genus. The MSS rankings were successfully linked to existing trait data in order to identify traits with predictive potential. Single traits as well as combinations of traits can be used to predict laboratory sensitivity to the substances tested, although associations were not as strong as in previous studies.

III) We also explore whether and in what ways traits can be linked purposefully to mechanistic effect models to predict intrinsic sensitivity using available data on the acute sensitivity and toxicokinetics of a range of freshwater arthropods exposed to chemicals, using the insecticide chlorpyrifos as an example. The results of a quantitative linking of seven different endpoints and twelve traits demonstrate that while quantitative links between traits and/or trait combinations and process based (toxicokinetic) model parameters could be established, the use of simple traits to predict classical sensitivity endpoints yields less insight. Future research in this area should include a quantitative linking of toxicodynamic parameter estimations and physiological traits, and requires further consideration of how mechanistic trait-process/parameter links can be used for prediction of intrinsic sensitivity across species for different substances in ERA.

Paul J. van den Brink

Paul J. Van den Brink is a professor of chemical stress ecology and works at the research institute Alterra and the Aquatic Ecology and Water Quality Management Group of Wageningen University, both belonging to the Wageningen University and Research centre. At Wageningen University Paul chairs the chemical stress ecology group which currently consists of himself, a PostDoc and 9 PhD students. For both affiliations, he is involved in supervising and executing international projects on the scientific underpinning of higher tier risk assessment procedures for contaminants. Recent research topics are the development of effect models (e.g. individual based, meta-population models and eco informatics, expert base models), Trait based Ecological Risk Assessment (TERA) and ecological risk assessment of chemicals in the tropics. Since 1995, Paul van den Brink has published over 100 peer reviewed papers, for two of which he won an international prize. He also co-edited five books. In 2006 Paul won the LRI-SETAC Innovative Science Award. He also organized and took part in many international workshops and courses. Paul van den Brink is presently a member of the SENSE research school (www.sense.nl), associate fellow of the Canadian River Institute and editor of the journal: ‘Environmental Toxicology and Chemistry’. He is also the past-president of SETAC (Society of Environmental Toxicology and Chemistry; www.setac.org) World and of SETAC Europe. Paul is also a honorary visiting professor at the University of York.

Field validation of species sensitivity distributions

Adam Peters
WCA Environment, UK

There is a requirement for quality standard derived under the WFD to be compared with evidence from field studies. The same principle can also be applied to any chemical substance for which a robust ecological threshold (e.g. PNEC) has been derived, for example through the derivation of a Species Sensitivity Distribution. Several different approaches towards performing these types of assessments are outlined, including examples of real assessments. The advantages and limitations of various assessment approaches are considered for both whole community assessments and assessments that are targeted at particularly sensitive organisms.

In order to evaluate relationships between metal exposures and benthic community metrics, the bioavailability of the metals must be calculated for each site. Several approaches can be taken towards the assessment of PNEC values, including simplistic assessments of ecological quality at different exposure levels and the derivation of limiting functions (comparable to a traditional dose response relationship). Assessments can be based on the whole community, subsets of the community, groups of taxa, or an individual taxon. Analyses based at the level of the whole community may lack the sensitivity to identify slight effects on particularly sensitive species or families. Reducing the diversity of organisms assessed increases the uncertainty in the assessment, particularly for reference based methods. Approaches towards the identification of those taxa that should be considered as sensitive to a particular pollutant will be considered.

A novel approach for bridging the gap between quality standards based on laboratory ecotoxicity studies and site-specific local aquatic communities is also outlined. This approach aims to take account of variation in the composition of ecological communities, and the effect that this may have on the sensitivity of the community to a particular pollutant. This is illustrated with an example for deriving site-specific thresholds for zinc in an area affected by historic mining activities.

Adam Peters

Adam Peters, PhD is a Principal Consultant at wca environment and an environmental chemist with over 10 years of experience in environmental consultancy, environmental regulation and academia. Adam has considerable expertise in the bioavailability of trace metalsHe has previously been responsible for management of environmental aspects of the Notification of New Substances scheme and the Existing Substances Regulations in the UK, and has recently been a regular attendee as an expert for metals-related issues at European Commission TCNES. He has been closely involved with the development of Environmental Quality Standards for both metals and organic chemicals, and the preparation of the Metals Environmental Risk Assessment Guidance (MERAG). Adam's main areas of expertise are in the assessment of environmental fate, behaviour, bioavailability and effects of trace metals in relation to the use of Biotic Ligand Models; environmental risk assessment of industrial chemicals; assessment of Persistent, Bioaccumulative and Toxic (PBT) substances; Hazard assessment of waste materials and their recovery; and development and validation of environmental quality standards.

Key Publications

Peters A, Simpson P, Moccia A. 2013. Accounting for both local aquatic community composition and bioavailability in setting site-specific quality standards for zinc. *Environmental Science and Pollution Research* (in press).

Peters A, Simpson P, Merrington G, Schleckat C, Rogevich-Garman E. 2013. Assessment of the effects of nickel on benthic macroinvertebrates in the field. *Environmental Science and Pollution Research* (in press).

Peters A, Lofts S, Merrington G, Brown B, Stubblefield W, Harlow K. 2011. Development of biotic ligand models for chronic manganese toxicity to fish, invertebrates, and algae. *Environmental Toxicology and Chemistry*, 30; 2407–2415.

Peters A, Crane M, Adams W. 2011 Effects of iron on benthic macroinvertebrate communities in the field. Bulletin of Environmental Contamination and Toxicology 86:591-595.

Crane M, Fisher B, Leake C, Nathail P, Peters A, Stubblefield W, and Warn T. (2010) How should an environmental standard be implemented. Chapter in: Derivation and Use of Environmental Quality and Human Health Standards for Chemical Substances in Water and Soil. SETAC CRC Press, Boca Raton, FL. 140 pp.

Derivation of toxicity thresholds for LAS – integration of QSARs, SSDs, mescosms, and field data

Scott Belanger
Procter & Gamble, USA

Linear alkylbenzene sulfonate (LAS) has been one of the most heavily used anionic detergent chemicals globally since its introduction to the market in the 1960's. As such, it has a rich information base spanning physical-chemical properties, specific analytical methods applicable to all environmental matrices, acute and chronic toxicity, bioaccumulation, field monitoring data, and assessments using stream mesocosms. In this talk, this information will be reviewed in support of an integrated approach that translates acute and chronic toxicity data on pure LAS materials and technical mixtures to field-relevant distributions of LAS leaving wastewater treatment plants (which does not bear a direct relationship to toxicity tests performed in the laboratory). Using the so-called toxicity normalization method, laboratory toxicity data will be re-presented in light of field distributions to generate robust Species Sensitivity Distributions (SSDs) that are probed to understand the singular robustness of the SSD itself. Leave-one-out and add-one-in Monte Carlo simulations are used to quantitatively and qualitatively evaluate "what-if" scenarios regarding the generation of additional data. Lastly, SSDs will be compared with robust stream mesocosm studies on LAS to support their predictive nature.

Scott Belanger

Scott Belanger is presently a Research Fellow in Procter & Gamble's corporate safety and sustainability organization where he has broad leadership responsibilities for environmental toxicology, science, and technology guidance from an environmental perspective. He holds degrees from the University of Wisconsin (B.S.), Bowling Green State University (M.S.) and Virginia Tech (Ph.D. and post-doctoral appointment). Prior to joining P&G in 1989, he was an Assistant Professor in Environmental Toxicology at the University of Louisiana-Lafayette. During his tenure at P&G Scott has directed research at P&G's Experimental Stream Facility in southwestern Ohio evaluating the ecological impacts of P&G's highest volume detergent chemicals. Later he assumed responsibility for P&G's global environmental toxicology function, leads efforts on environmental animal alternatives and has overall responsibility for management of P&G's corporate human and environmental safety research portfolio. Scott is a recognized authority in the responses of aquatic life to man-made and natural stressors and has authored over 100 published scientific articles, books and book chapters on these topics. He has served on numerous national and international panels providing advice to organizations such as the U.S. Environmental Protection Agency, the OECD (Organization for Economic Co-operation and Development, an international governing body), the European Commission, the Japanese Ministry of Environment, Trade and Industry, and Environment Canada.

Presently in P&G's Corporate Environmental Safety and Sustainability Organization he directs research on ecological and toxicological responses of fish, invertebrates and algae to consumer product chemicals and advises P&G broadly on the development of new technologies and issues relating to environmental matters

Field-based species sensitivity distribution and community sensitivity distribution as alternative ways for field validation of the PNECs derived from laboratory based approaches

Kenneth Mei Yee Leung
The Swire Institute of Marine Science and School of Biological Sciences, The University of Hong Kong, Hong Kong, China

The determination of predicted no-effect concentrations (PNECs) and sediment quality guidelines (SQGs) of toxic chemicals in marine sediment is very crucial in ecological risk assessment, sediment quality management (e.g. mud disposal in the sea) and environmental remediation (e.g. dredging of contaminated mud). However, current methods of deriving sediment PNECs are primarily based on toxicity data generated from laboratory ecotoxicity bioassays that are often lack of ecological realism. To tackle this issue, we have developed two novel alternative approaches to scientifically derive site-specific SQGs by utilizing field data of benthic biodiversity and contaminant concentration which are concurrently measured in sediment samples collected from the area of concern. In this talk, I will first describe the principle of these field-based approaches. Secondly, I will introduce the field-based species sensitivity distributions (f-SSDs) approach, which is based on the relationship between species abundance and contaminant level [Environmental Science & Technology 39:5148-5156; Environmental Toxicology & Chemistry 27:226-234]. Since its establishment, f-SSDs have been utilised in different parts of the world such as Europe, Hong Kong, New Zealand and the United States. Norwegian continental shelf and the marine environment of Hong Kong will be taken as examples to illustrate the methodology. Thirdly, I will present the community sensitivity distributions (CSDs) approach which is founded on the relationship between species density and contaminant level, and makes use of Empirical Bayes methods [Environmental Science & Pollution Research 21: 177-192]. Overall, the field-data-derived SQGs appear to be more environmentally relevant and ecologically realistic. The f-SSD and CSD can be directly adopted as 'effect distributions' for probabilistic risk assessment. The field-data-derived SQGs can be employed as site-specific guidelines, and used to validate the current PNECs or SQGs derived from laboratory ecotoxicity data. Finally, the limitation of these field-based approaches will be discussed, while their recent development and application in different countries will be highlighted.

Kenneth Leung

Kenneth Leung is Professor of Aquatic Ecology and Toxicology at the Swire Institute of Marine Science and School of Biological Sciences, in the University of Hong Kong (HKU), Hong Kong, China. Currently, he is also serving as Associate Dean (Research and Graduate Studies) at the Faculty of Science in HKU. During 2010–2012, he was the elected President of the Society of Environmental Toxicology and Chemistry (SETAC) Asia Pacific Geographic Unit.

Kenneth Leung obtained a BSc degree in Applied Environmental Sciences with first class honours at University of Portsmouth in England in 1993, and accomplished his MPhil study in Environmental Science at City University of Hong Kong in 1996. As a recipient of the Swire's James Henry Scott PhD Scholarship, he undertook a doctorate study at University of Glasgow in Scotland and obtained his PhD in marine ecotoxicology in 2000. He was subsequently awarded the Croucher Foundation Fellowship, enabling him to conduct his 18-month postdoctoral study in ecological risk assessment of antifouling biocides at Royal Holloway, University of London in England (2000-2001). He firstly joined HKU as Research Assistant Professor in January 2002 and was promoted to Assistant Professor, Associate Professor (Tenured) and Professor in 2003, 2009 and 2013, respectively.

Kenneth Leung is an aquatic ecotoxicologist with sound knowledge in aquatic ecology, biostatistics and ecological risk assessment (ERA). Since 1999, he has written or co-authored over 100 peer-reviewed articles which are principally related to the ecology, pollution, ecotoxicology and ERA in both marine and freshwater ecosystems. His current research projects include the derivation of water and sediment quality guidelines of chemical contaminants for protecting aquatic ecosystems, and development of statistical methods and models for predicting environmental risks of different chemicals and their mixtures. Since 2010, he has been assisting the Government of the Hong Kong Special Administrative Region to review the marine water quality objectives for various physical and chemical parameters. He is also a subject editor for the SETAC journal *Integrated Environmental Assessment and Management*, and serves as an editorial board member for six international journals including *Environmental Science and Pollution Research*, *Marine Pollution Bulletin*, *Integrative Zoology*, *Canadian Journal of Zoology*, *Ocean Science Journal* and *Toxicology and Environmental Health Science*. He is the leading guest editor for a special volume entitled "*Environmental quality benchmarks for protecting aquatic ecosystems*" which has been published in *Environmental Science and Pollution Research* in January 2014 (*ESPR* 21:1-243).

Over the past, Kenneth Leung was invited by the Food and Agriculture Organisation to develop a manual for assessing ecological risks of aquaculture practices, and frequently invited by the United Nations (UNDP/PEMSEA) to give lectures on ERA-related topics in regional training workshops. He was a recipient of the "*Marine Pollution Bulletin Highly Cited Author Award [2005-2009]*" by Elsevier, the "*Award for Service Contribution 2010*" by Faculty of Science, HKU and "*2012 Outstanding Alumni Award*" by Vocational Training Council of Hong Kong. Owing to his professional achievements and community services, Kenneth Leung was selected as one of the "*Ten Outstanding Young Persons*" for Hong Kong by Junior Chamber International in 2010.

HC5 estimation in SSDs revisited

Tom Aldenberg
RIVM,the Netherlands

Species Sensitivity Distributions (SSDs)–in their basic form defined as univariate continuous statistical distributions over a logarithmic species sensitivity concentration axis for a particular chemical substance–can be applied in environmental risk assessment to estimate a PNEC (Predicted No-Effect Concentration) for that toxicant. This PNEC is in many cases implemented as a statistical estimate of the log HC5 concentration. This minimalist model, originally due to Kooijman and Van Straalen, needs extension to address a multitude of thinkable challenges, e.g. with regard to species selection, ecosystem representativeness/ functioning, data quality, statistical model selection, and predictive evaluation of the SSD and its quantiles. In this paper, we will first review how we handled the uncertainty of the log HC5 for the Logistic and Normal distribution, from a Bayesian viewpoint. Second, we develop the estimation of the so-called *predictive distribution*–formally the mean of the Bayesian spaghetti plot SSD–in order to pinpoint a single-curve SSD for a given statistical family. This leads to an *improved log HC5*–or other quantile–estimate, to better reflect uncertainty due to small sample size. Presently, we consider the ubiquitous median estimate log HC5 as being unrealistically insensitive to small sample size, hence risking lack of conservativeness. This is compounded by the 5^{th} and 95^{th} confidence limits of log HC5 uncertainty often not being reported. The Bayesian predictive distribution method spawns *a new table of extrapolation constants*, addressing both chronic and acute species sensitivity data, depending on the basic fraction affected. The sensitivity of these new extrapolation constants is evaluated in the light of the REACH-required samples sizes of 10, preferably 15. A recurring concern is the effect of log species toxicity *data uncertainty*. Operationally, this may derive from having multiple data for the same species, from *dose-response curve confidence limits*, from *QSAR-estimated toxicity data* with associated confidence, and possibly a host of other sources of uncertainty. Intuitively, one would expect data uncertainty to further lower old–as well as new–log HC5 estimates, but methods of hierarchical modelling reveal that the reverse is the case: the more variation has to be attributed to the individual species points, the less variation remains for the SSD itself. Surprisingly, theory, as well as numerical experiments, show that *the effect of data uncertainty is quite modest*, leading to the recommendation to take the mean of log data point uncertainty, and continue with the old, or updated, extrapolation methodology, *as if data were certain*. Averaging multiple species data was already REACH-recommended. It follows that using such averages per species, or employing point estimates, i.e. expected values, through model-estimated species sensitivities, only leads to slightly increased conservative–that is lower–estimates of PNEC values pursued. Both new insights of predictive SSD and the effect of data uncertainty would somewhat alleviate the need for assessment factors addressing these particular issues.

Tom Aldenberg

Tom Aldenberg has been working as a bio-mathematician for over 30 years. He graduated as a fisheries biologist at the University of Amsterdam and studied Theoretical Biology in Leiden and Applied Mathematics in Amsterdam. Tom has worked at RIVM since 1979 and is employed as Senior Scientist. In the first part of his career, he specialized in ecosystem modeling: nutrient and species dynamics in eutrophic lakes, and trophic transfers of toxicants in aquatic and terrestrial foodwebs. In the second part of his career, attention shifted to Species Sensitivity Distribution (SSD) modeling, a statistical technique involving Bayesian statistics, to derive Hazardous Concentrations and Fraction of species Affected from species toxicity data. He worked on Probabilistic Environmental Risk Assessment and participated in CEFIC, EFSA, and EUFRAM EU-based projects by contributing techniques to estimate Expected Risk. Expected Risk is an improvement of the Risk Characterization Ratio (RCR), which is the basis of REACH-based Guidance to evaluate the risk of chemicals. Recently, he has been participating in the EU projects: OSIRIS and CADASTER. In OSIRIS, Tom has built models for analyzing the information content and methods of decision making in Repeated Dose toxicity studies, and has developed models for categorical data to quantify the statistical Weight-of-Evidence in Integrated Testing Strategies (ITSs) of Mutagenicity, Carcinogenicity, and Skin Sensitization. Several co-authored publications on this have been published in Regulatory Toxicology and Pharmacology. In CADASTER, he has studied methods to build SSDs from QSAR-generated species data. This introduces data uncertainty into the SSD, which basically requires hierarchical Bayesian modeling. Recent interests are probabilistic decision trees, information-based model selection and confirmation measures in automated reasoning.

Two SSD-related publications, cited 500 and 250 times, respectively:

T Aldenberg, W Slob (1993). Confidence limits for hazardous concentrations based on logistically distributed NOEC toxicity data. *Ecotoxicology and Environmental Safety*, 25 (1), 48-63.

T Aldenberg, JS Jaworska (2000). Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. *Ecotoxicology and Environmental Safety*, 46 (1), 1-18.)

Assessment factors for deriving PNECs: Food for thought

Ad M.J. Ragas
Radboud University,the Netherlands

Within regulatory contexts such as REACH and the European Water Framework Directive (WFD), assessment factors are used to derive safe exposure levels for aquatic and terrestrial ecosystems from single species toxicity data. These safe exposure levels are also referred to as Predicted No Effect Concentrations or PNECs. If toxicity data are available for a limited set of aquatic species – e.g. an alga, a daphnia and a fish – the lowest value is typically divided by an assessment factor to arrive at the PNEC. The value of this assessment factor varies between 10 and 1000, depending on the number and the nature of the available data. If chronic NOECs are available for an extensive set of aquatic species (i.e. > 15 species covering at least 10 different taxonomic groups), the 5th percentile of the species sensitivity distribution (SSD) is determined and an assessment factor of 1-5 is subsequently applied to arrive at the PNEC. The main aim of the current contribution is to formulate recommendations for improving the use of assessment factors in deriving PNECs. These recommendations are based on a statistical analysis of a large set of chronic toxicity data resulting from aquatic single species tests and mesocosm experiments.

A database with chronic single species NOECs on 20 different chemicals was compiled based on data reported in the open literature. Chronic mesocosm data were found for 6 of these substances and were also included in the database. For each of the substances in the database, the 5th percentile of the SSD (HC_5) was determined. This HC_5 was then compared with:

- the PNEC reported in the mesocosm experiments (if available);
- PNECs derived by applying a safety factor of 10 to the lowest value of a limited dataset of 3, 6 or 9 NOECs. These datasets were generated by parametric bootstrapping of the available single-species NOECs.

Mesocosm PNECs were generally lower than the HC_5, with two notable exceptions, i.e., lindane and dimethoate, which can be explained by the limited set of species in the mesocosm. The HC_5 is on average a factor of 2.0 lower that the PNEC derived from a set of 3 chronic NOECs. This difference increases to a factor of 4.5 and 7.2 for datasets with 6 and 9 chronic NOECs, respectively. Based on these results two general recommendations are formulated:

- The assessment factor of 10 that is currently being applied to the lowest value of small datasets (i.e. alga, daphnid and fish) should be differentiated depending on the number of available data, e.g. a factor of 20 if one value is available for each taxonomic group, but a value of 5 when three or more values are available for each taxonomic group.
- The default assessment factor of 2 is suggested for the HC5 of the SSD. This default value can be further refined based on the specific characteristics of the available toxicity data, i.e. representativeness, mode of action, interspecies variability and uncertainty.

Ad M.J. Ragas

Ad Ragas studied biology and obtained a PhD degree at the Radboud University in Nijmegen. He currently holds a position as an assistant professor at the Department of Environmental Science at the Radboud University in Nijmegen, and as a full professor in Environmental Sciences at the School of Science at the Open Universiteit in Heerlen, The Netherlands. His main domain of expertise is the modelling of human and environmental risks of chemical substances, covering areas such as fate and exposure modelling, effect modelling, chemical mixtures, integration of human and ecological risk assessment and risk perception. Within this domain, his focus is on uncertainty assessment and dealing with uncertainties in decision-making. He coordinates a work package on risk assessment of pharmaceuticals in the EU FP7 PHARMAS project. He is deeply involved in academic educational programmes for environmental scientists, i.e. as a coordinator of an MSc programme in Environmental Sciences and of several specific courses, e.g. in risk assessment, GIS and statistics. He chairs the Dutch scientific advisory committee on quality standards for air and water.

Selected recent publications:

Løkke H, Ragas AMJ, Holmstrup M. 2013. Tools and perspectives for assessing chemical mixtures and multiple stressors. *Toxicology* (in press).

Oldenkamp R, Huijbregts MAJ, Hollander A, Versporten A, Goossens H, Ragas AMJ. 2013. Spatially explicit prioritization of human antibiotics and antineoplastics in Europe. *Environment International* 51:13–26.

Ragas AMJ, Oldenkamp R, Preeker NL, Wernicke J, Schlink U. 2011. Cumulative risk assessment of chemical exposures in urban environments. *Environment International* 37:872–881.

Ragas AMJ, Brouwer FPE, Büchner FL, Hendriks HWM, Huijbregts MAJ. 2009. Separation of uncertainty and interindividual variability in human exposure modeling. *Journal of Exposure Analysis and Environmental Epidemiology* 19:201-212.

Weight of evidence approaches for deriving HC5s

Sandrine Andres
INERIS, France

Experience gained in developing Quality Standards (e.g. PNEC) in the framework of the EU Technical Guidance Document shows that only a few substances can benefit from the use of an Species Sensitivity Distributions (SSD), even if substances appears after an initial assessment as data rich substances. The main drawback is the lack of validated studies for the additional taxa. Indeed, the level of standardisation for testing these additional taxa (such as mayfly, dragonfly, amphibian, rotifer, molluscs, etc...) is usually lower than for the regular algae/daphnid/fish simplified trophic chain. As a consequence, this additional information is often not used for the assessment.

In order to make the best use of all the information available, a Multi-Criteria Decision Analysis (MCDA) tool was developped in the framework of the research project AMORE (Multi-Criteria Analysis for the Development of a Decision Support Tool for the prevention of Environmental Risks). This tool is based on Weight of Evidence (WoE) methodology, which aims to improve the evaluation of ecotoxicological data, through the assessment of their relevance and reliability for the definition of SSDs. The methodology allows to rank the acceptability of ecotoxicological data for further use in the risk assessment process and therefore optimise their influence in the production of reliable SSDs, through a weighted bootstrap modelling procedure for data resampling.

In this project, it was hypothetised tha the SSD can be based on all avaialble ecotoxicity data, which can be heterogeneous and often non comparable. These data can be obtained through different approaches (e.g. experimental or even modelling) and conditions, e.g., the protocol can be standardized or not; time duration can vary among experiments, leading to chronic or acute data; different physiological endpoints can be observed, e.g. mortality, growth, reproduction; statistics used for interpreting data can differ, e.g. leading to NOEC or ECx.

The methodology is based on the assessment of a hierarchically structured set of 57 criteria, which is used for assigning a quantitative score to every ecotoxicological datum and was created based on the review of the state of the art frameworks for the assessment of ecotoxicological data. The different endpoints are analysed based on their production method and specifically on three main aspects: the 'Experimental Reliability', the 'Statistical Reliability' and the 'Biological Relevance' of the experimental or modelling protocol used. This assessment has been developed in with the contribution of an expert panel of scientists on ecotoxicology. Knowledge and preferences of experts have been gathered through a participatory process, and is used for the calculation of the aggregated reliability scores of data. The nature of the process mandates the use of Fuzzy Logic during the aggregation phase, for handling the inherent uncertainty which appears in the form of unreported information, as well as possible lack of knowledge of the experts. This approach allows for a weighed use of the available information available in a weight of evidence perspective.

Sandrine Andres

Sandrine ANDRES, PhD, is the head of Unit “Evaluation and Expertise in Toxicology” at INERIS (National Institute for the Industrial Risks and the Environment). She holds a PhD in “Environmental toxicology” from the University of Toulouse III. She also pursued a postdoctoral research mainly focusing on Mercury absorption through biological membranes. (University of Maryland, USA). Prior to join INERIS, Sandrine worked as Consultant as risk assessment expert, where one of her main task was in support to the EU Commission for the implementation of the Rotterdam Convention.

At INERIS, she worked from 2006-2009 as coordinator of the technical evaluation of the dossiers in the framework of the Biocidal Product Directive. Currently, the activities of the Unit mainly take place within the regulatory frameworks of REACH, CLP, and the Water Framework Directive. This Unit is in charge *inter alia* of the development of Environmental Quality Standard (EQS) at National level and works on scientific issues related to the implementations of those EQS. She participates to several national and international experts groups including, Member of the POP-Review Committee (Convention de Stockholm) (UNEP) since 2007, Member of the Task Force Biocides (OECD) since 2006, Member of the Task Force « Environmental Exposure Assessment » (OECD.) since 2007. Current interests include the improvement of methodologies in support to environmental risk assessment of chemicals, both from an Hazard and Exposure assessment perspective.

ABSTRACT

Sample size in PNEC derivation

Scott Dyer
Procter & Gamble, USA

SSDs have been used to develop water quality criteria (e.g., PNECs) and other protective environmental concentrations (e.g., HC5). These criteria typically require large datasets (e.g., USEPA ambient water quality criteria utilize at least 8 acute toxicity values from several taxa spanning three trophic levels, fish, invertebrates and plants) of measured toxicity values. However, there has been a considerable debate regarding the minimum requirements for establishing protective concentrations, such as the HC5, within the scientific and regulatory communities. For organizations needing to establish these criteria, questions remain whether the addition of taxa into the SSD will greatly change the criterion. Is it possible that the addition of taxa will not change the HC5 and thereafter the PNEC? Is there a law of diminishing returns for expanding the number of taxa incorporated into an SSD? If so, then understanding factors that dictate the lack of need for additional taxa would result in appropriate PNECs without undo cost and time. To explore this question we developed distributions with steep to shallow scale (slope) factors as well as small to large toxicity ranges. Within these diverse distributions we assessed the effect of the numbers of taxa values included to generate HC5 values as well as their position within the distribution. Comparisons of these distributions to real chemical datasets will be discussed.

Scott Dyer

Scott D. Dyer obtained his B.S. and M.S. degrees from Iowa State University in Biology and Toxicology, respectively. His Ph.D. was awarded from the University of North Texas where he studied the stress protein response in fish exposed to diverse contaminants via laboratory and field exposures. Since 1991, Dyer has been employed by The Procter & Gamble Company (P&G), Cincinnati, Ohio, and is presently a Principal Scientist in the Environmental Stewardship Organization as an eco-toxicologist. His primary mission within P&G is researching methods that advance the predictions of potential environmental exposure and effects of chemicals found in consumer products. He currently has three major research programs, all collaborations with academia, government and industry: 1) the eco-epidemiology of consumer product chemicals relative to other chemical and physical stressors; 2) the extrapolation of potential effects across species; and 3) the development of screening tools for the estimation of metabolism in fish, an important attribute for the prediction of bioaccumulation. Dyer has authored more than 70 journal articles, book chapters, and technical reports and currently participates with work groups within organizations such as the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Environment & Health Risk Assessment and Management (ERASM), American Cleaning Institute (ACI), Water Environment Research Foundation (WERF), ILSI Health and Environmental Sciences Institute (HESI) and the Society of Environmental Toxicology and Chemistry (SETAC). He currently serves on the Board of Directors for WERF and Confluence, a water technology innovation cluster in Cincinnati, Ohio, USA.

ABSTRACT

How to extrapolate across 100,000+ substances, sites and species with SSDs?

Jan Hendriks
Radboud University, the Netherlands

Each second, one new chemical is added to the more than 65,000,000 already registered. In the EU, 100,000+ compounds are awaiting assessment while 1,500,000 contaminated sites potentially require cleanup. Worldwide, 8,000,000+ species, of which 10,000+ endangered, need protection (Hendriks 2013).

At the same time, empirical research is severely limited by financial, practical and ethical constraints. Assessing 100,000+ substances at 100,000+ sites threatening 100,000+ species obviously cannot be achieved by toxicological testing only. As an alternative, I suggest to focus on simple models. Instead of going for statistical regressions with the highest explained variability, we might attach more value to meaningful equations of which the coefficients and exponents can be interpreted physically.

We have derived and collected SSDs on toxic and non-toxic stressors to discern patterns across stressors, species and endpoints. In this contribution, some examples will be discussed. We will look at (1) intra-species and inter-species variability, (2) the number of species included in an SSD, (3) SSDs across modes of action, (4) the combined use of SSDs for toxic and non-toxic stressors, (5) "field"-based SSDs (PNOFs) and (6) in vitro biomarker SSDs to in vivo bioassay SSDs (References given below).

Azevedo LB, Van Zelm R, Elshout PMF, Hendriks AJ, Leuven RSEW, Struijs J, De Zwart D, Huijbregts MAJ. (2013) Species richness – phosphorus relationships for lakes and streams worldwide. *Global Ecology and Biogeography*, in press.

De Hoop L, Smit M, Huijbregts MAJ, Leuven RSEW, Schipper AM, Hendriks AJ (2011). Sensitivity of arctic species to oil and other contaminants in comparison to other species, *Environmental Science and Technology* 45: 9017–9023.

Elshout PMF, Dionisio Pires LM, Leuven RSEW, Wendelaar Bonga SE, Hendriks AJ (2013). Low oxygen tolerance of different life stages of temperate freshwater fish species. *Journal of Fish Biology* 83: 190-206.

Fedorenkova A, Lenders HJR, Ouborg J, Breure AM, Hendriks AJ (2010). Ecotoxicogenomic: bridging the gap from genes to population, *Environmental Science and Technology* 44: 4328-4333

Fedorenkova A, Vonk JA, Lenders HJR, Creemers R, Breure AM, Hendriks AJ (2012). Ranking ecological risks of multiple chemical stressors on amphibians, *Environmental Toxicology and Chemistry* 31: 1-6.

Fedorenkova A, Vonk JA, Breure AM, Hendriks AJ, Leuven RSEW (2013). Tolerance of native and non-native fish species to chemical stress: a case study for the river Rhine. *Aquatic Invasions* 8: 231–241.

Golsteijn L, Van Zelm R, Hendriks AJ, Huijbregts MAJ (2013). Statistical uncertainty in hazardous terrestrial concentrations estimated with aquatic ecotoxicity data. *Chemosphere* 93: 366–372.

Golsteijn L, Van Zelm R, Veltman K, Musters G, Hendriks AJ, Huijbregts MAJ (2012). Including ecotoxic impacts on warm-blooded predators in Life Cycle Impact Assessment. *Integrated Environmental Assessment and Management* 8: 372–378.

Hendriks AJ (2013). How to deal with 100,000+ substances, sites, and species: Overarching principles in environmental risk assessment. *Environmental Science and Technology* 47: 3546−3547.

Hendriks AJ, Awkerman JA, De Zwart D, Huijbregts MAJ (2013). Sensitivity of species to chemicals: differences between test types (LC50, LD50), cold-blooded and warm-blooded species and modes of action. *Ecotoxicology and Environmental Safety* 97: 10-16.

Smit MGD, Bechman RK, Hendriks AJ, Skadsheim A, Larssen BK, Baussant T, Bamber S, Sanni S (2009). Relating biomarkers to whole-organism effects using species sensitivity distributions: a pilot study for marine species exposed to oil. *Environmental Toxicology and Chemistry* 28: 1104–1109.

Jan Hendriks

Interests

- 1000^+ physical-chemical pressures → 1000^+ biological impacts
- chemistry - toxicology - (macro-)ecology, in particular chemokinetics – ecotoxicodynamics
- cycling of (xeno-)biotic constituents using overarching principles at cell - landscape level

Employment

- 2004-… Professor/Head, Dep. Environmental Science, Radboud University Nijmegen, NL
- 1999-04 Section Head, Dep. Chemistry and Ecotoxicology, RIZA/Deltares, Lelystad, NL
- 1990-99 Scientist-Advisor, Section Ecotoxicology, RIZA/Deltares, Lelystad, NL
- 1988-89 Scientist-Advisor, Dep. Ecology and Management, TNO, Delft, NL.

Supervision and publications

- (Co-)supervisor of 30^+ P(h)Ds and 30^+ MScs
- (Co-)author of 130 international peer reviewed articles and 60 (chapters in) reports & books

Info and publications

- http://www.ru.nl/environmentalscience/, http://www.ru.nl/environmentalscience/publications/
- http://www.ru.nl/environmentalscience/staff/individual-staff/hendriks/

Key publications (Species Sensitivity Distributions)

The publications below are in addition to the presentation references on the previous page.

Azevedo LB, van Zelm R, Hendriks AJ, Bobbink R, Huijbregts MAJ (2013). Global assessment of the effects of soil acidification on plant species richness, *Environmental Pollution* 174: 10-15.

Azevedo LB, De Schryver A, Hendriks AJ, Huijbregts MAJ (2014). Calcifying species sensitivity distributions for ocean acidification. *Marine Pollution Bulletin* submitted.

Leuven RSEW, Hendriks AJ, Huijbregts MAJ, Lenders HJR, Matthews J, Van der Velde G (2011). Differences in sensitivity of native and exotic fish species to changes in river temperature. *Current Zoology* 57: 852−862.

ABSTRACT

Interspecies Correlation Estimation (ICE) Models predict supplemental toxicity data for SSDs

Sandy Raimondo
Environmental Protection Agency, USA

Species sensitivity distributions (SSD) require a large number of toxicity values for a diversity of taxa to define a hazard level protective of multiple species. For most chemicals, measured toxicity data are limited to a few standard test species that are unlikely to adequately represent ecological communities. Interspecies correlation estimation (ICE) models are log-linear least squares regressions that predict the acute toxicity to untested taxa from known toxicity of a single surrogate species. A suite of ICE models is developed from a comprehensive, standardized dataset of acute toxicity with the goal of maximizing the number of potential species for which toxicity can be predicted while minimizing extraneous sources of variation in the models. The United States Environmental Protection Agency houses three ICE databases: aquatic animals (vertebrates and invertebrates; 5501 records, 180 species; 1266 chemicals), algae (1647 records, 69 species, 457 chemicals), and wildlife (birds and mammals; 4329 records, 156 species, 951 chemicals). Approximately 2400 models have been developed from these databases and made available through the Web-based Interspecies Correlation Estimation internet application (Web-ICE; http://epa.gov/ceampubl/fchain/webice/). ICE models were validated using leave-one-out cross validation and sources of model uncertainty evaluated. Toxicity predictions are most accurate for models with closely related taxa pairs, with over 90% of cross-validated values predicted within 5-fold of the measured value when the surrogate and predicted taxa are in the same family. Model mean square error and prediction confidence intervals should be considered when evaluating an ICE predicted value. Models built with a single mode of action (MOA) were often more robust than models built using toxicity values with multiple MOAs, and improve predictions among species pairs with large taxonomic distance (e.g., within phylum). SSDs developed solely from ICE-predicted toxicity values produce hazard levels with an average factor of 3.0 and 5.0 of those developed with all measured data for aquatic species and wildlife, respectively. For chemicals in which more measured data are available, ICE models may be used to augment datasets to increase species diversity in SSDs. Compared to SSDs developed from only measured data, the uncertainty of ICE model predictions contributes less variability to hazard levels than variance due to species composition. Through extensive study of ICE model evaluation and uncertainty and their application in developing SSDs, ICE generated toxicity values have been demonstrated to provide a statistically sound approach to supplementing datasets to generate SSD-based hazard levels applicable to ecological risk assessments.

Sandy Raimondo

Dr. Raimondo currently serves as a Supervisory Research Ecologist of the Biological Effects and Population Response Branch within the United States Environmental Protection Agency (US EPA) Gulf Ecology Division. She has been with the US EPA for over 10 years with focused research areas that include: the development of models that predict ecological effects of environmental stressors on organisms, populations, and ecosystems; survival and recruitment modeling; aquatic toxicity tests; dose-response relationships; toxicity extrapolation modeling; toxicity estimation; uncertainty analyses of complex ecological processes; aquatic & coastal ecosystems; ecological risk assessment. Sandy led the development of the Interspecies Correlation Estimation (ICE) modeling tool, Web-ICE (http://www.epa.gov/ceampubl/fchain/webice/index.htm), which predicts acute sensitivity of toxicants to aquatic species and wildlife. Web-ICE is used by EPA Regions and Program Offices to establish water quality and pesticide registration policy. A recent update to Web-ICE (April 2013) includes new ICE models predicting toxicity of algal taxa and improved functionality of Species Sensitivity Distribution (SSD) and Endangered Species Modules. Sandy also leads the development of spatially-explicit models that evaluate the effects of environmental stressors on populations and ecosystems with focus on uncertainty and complexity of ecological processes. Sandy has published over 50 peer-reviewed publications, book chapters, and technical reports, including 11 publications in high impact journals on ICE modeling and their application in supplementing data to develop SSDs. She has delivered over 10 seminars and short courses on Web-ICE at international conferences, as well as regular technical training to US EPA Program Offices and Regions. She has received over 25 awards within EPA, including an Agency bronze medal and Office of Research and Development Impact Award for the development of Web-ICE.

Demonstration of the Web-Based Interspecies Correlation Estimation (Web-ICE) Modelling Application

Sandy Raimondo
Environmental Protection Agency, USA

The Web-based Interspecies Correlation Estimation (Web-ICE) modeling application is available to the risk assessment community through a user-friendly internet platform (http://epa.gov/ceampubl/fchain/webice/). ICE models are log-linear least square regressions that predict acute toxicity (LC50/LD50) of a chemical to a species, genus, or family based on estimates of relative sensitivity between the taxon of interest and that of a surrogate species. Web-ICE v 3.2 includes over 1440 models for aquatic animal taxa, 100 models for algae, and 852 models for wildlife taxa. Web-ICE has modules that predict toxicity to one taxa of interest at a time while providing detailed information on model parameters. It also has Species Sensitivity Distribution (SSD) and endangered species modules that produce toxicity values to multiple species based on the number of surrogates entered. In the SSD module, a user can enter up to 20 surrogate species which are used to predict toxicity to all predicted taxa possible. The entered surrogate and predicted toxicity values are used to develop a log-logistic probability distribution and estimate a hazard level equivalent to either the 1st, 5th or 10th percentile of the distribution. Users can also enter multiple surrogate toxicity values into the endangered species module, which are used to calculate predicted species, genus, and family level sensitivity for selected endangered species. Both the SSD and endangered species modules provide exportable data files of predicted results. A demonstration of the Web-ICE will familiarize participants with the functionality of the application and provide examples of its use for single taxon predictions, SSD generation, and development of endangered species toxicity reports.

Sandy Raimondo

Dr. Raimondo currently serves as a Supervisory Research Ecologist of the Biological Effects and Population Response Branch within the United States Environmental Protection Agency (US EPA) Gulf Ecology Division. She has been with the US EPA for over 10 years with focused research areas that include: the development of models that predict ecological effects of environmental stressors on organisms, populations, and ecosystems; survival and recruitment modeling; aquatic toxicity tests; dose-response relationships; toxicity extrapolation modeling; toxicity estimation; uncertainty analyses of complex ecological processes; aquatic & coastal ecosystems; ecological risk assessment. Sandy led the development of the Interspecies Correlation Estimation (ICE) modeling tool, Web-ICE (http://www.epa.gov/ceampubl/fchain/webice/index.htm), which predicts acute sensitivity of toxicants to aquatic species and wildlife. Web-ICE is used by EPA Regions and Program Offices to establish water quality and pesticide registration policy. A recent update to Web-ICE (April 2013) includes new ICE models predicting toxicity of algal taxa and improved functionality of Species Sensitivity Distribution (SSD) and Endangered Species Modules. Sandy also leads the development of spatially-explicit models that evaluate the effects of environmental stressors on populations and ecosystems with focus on uncertainty and complexity of ecological processes. Sandy has published over 50 peer-reviewed publications, book chapters, and technical reports, including 11 publications in high impact journals on ICE modeling and their application in supplementing data to develop SSDs. She has delivered over 10 seminars and short courses on Web-ICE at international conferences, as well as regular technical training to US EPA Program Offices and Regions. She has received over 25 awards within EPA, including an Agency bronze medal and Office of Research and Development Impact Award for the development of Web-ICE.

HC5s from taxonomically structured hierarchical species sensitivity distributions

Peter Craig
Durham University, UK

One approach to deriving the predicted no-effect concentration for a chemical is to use a species sensitivity distribution (SSD) model to estimate the hazardous concentration affecting p% of species (HCp), where p is usually 5. Many questions have been raised about both principles and application of SSDs but the concept has nevertheless been found to be useful.

Analysis of a database of aquatic ecotoxicity test results reveals a number of features which should be addressed by SSD methodology. These include: inter-species correlation; tendencies of particular species to one or other end of the sensitivity distribution; and inter-test variation. In earlier work, attempts have been made at addressing each of these issues on its own. Addressing them collectively requires multivariate statistical modelling.

We present a Bayesian hierarchical model of variability and uncertainty for sensitivities of species to a chemical undergoing assessment and for a database of relevant test results for other chemicals. The Bayesian approach has several advantages over traditional non-Bayesian statistical methodology aimed primarily at analysing experimental data. It can incorporate both data and other information such as expert judgements or results of meta-analyses. It provides a collective description of uncertainty for all components of a model, a coherent mechanism for revising uncertainty when additional data become available, and a decision-making framework which addresses both uncertainty and utility.

Our model generalises the single randomly-sampled-chemical model proposed by Aldenberg and Jaworska (2000) and addresses the issues raised above. It models inter-species correlation by building species tendencies and sensitivities hierarchically, based on the taxonomic classification of species. Taxonomically-related structure seems natural and makes the model a better description of the available data but means that it is necessary also to specify a taxonomic scenario: the taxonomic structure of the community being protected by the HCp. The HCp is then scenario-specific, being the pth percentile of sensitivity to the chemical for species in the scenario. The Bayesian nature of the model means that the HCp estimate is automatically accompanied by a quantitative assessment of uncertainty.

The model is available in software form for application to test data for a new chemical. The software, known as hSSD, will be demonstrated at the workshop and is one of the methodologies used in the workshop case studies.

Peter Craig

My undergraduate degree was in Mathematics from Trinity College Dublin and was followed by a PhD in statistics and a two-year postdoctoral position studying the use of satellite imagery in the search for mineral deposits, both in TCD with a one year visit to the University of Washington. Since 1989, I have been a lecturer and then senior lecturer in statistics at Durham University, active in teaching, research, consultancy and IT management and tools.

I have a wide ranging expertise in statistical methodology and applications, especially in Bayesian modelling and related computation. In the 1990s, I was part of the group at Durham leading the way in statistical methodology for analysis of uncertainty for computer models of natural phenomena, especially oil reservoir models. Since 2004, initially as external expert contributing to European Food Safety Authority scientific opinions, I have been active in various areas of risk assessment including dietary exposure to pesticides, ecotoxicology and margins of exposure for carcinogens. My principal interests in risk assessment are improved modelling, in particular of chains of evidence, better quantification of uncertainty for risk assessment procedures and methodology for partial quantification of uncertainty based on limited specifications by experts. I have published in many of the best journals in the area of statistical methodology and more recently in journals such as Risk Analysis, Environmental Toxicology and Chemistry and Food and Chemical Toxicology.

I believe passionately in the importance of the mathematics underlying statistical reasoning but also that statisticians must devote a lot of time to exploring and analysing data and must engage at length and in depth with scientists in order to make a meaningful applied contribution.

Regulatory applications of SSDs in European regulations

Paul Whitehouse
Environmental Agency, UK

Regulatory frameworks like the Water Framework Directive, Marine Strategy Framework Directive and REACH are far-reaching pieces of legislation that require us to identify and manage pressures on the environment, including toxic chemicals. Assessing the hazard posed by chemicals is central to chemical risk assessment and also to the derivation of Environmental Quality Standards (EQSs) which play a key role in identifying risks and helping manage emissions to ensure wildlife and human health are not adversely impacted.

This presentation focuses on the role of EQSs in the Water Framework Directive. There have been important technical developments in the derivation and application of EQSs in recent years, some of which have been captured in EU Technical Guidance that was published in 2012. Whilst deterministic methods for deriving EQSs remain the only option in some cases, species sensitivity distributions (SSDs) are now widely used to derive EQSs, including standards for bioavailable metals and, in some cases, for biota standards. I will briefly review the experience of Member States in using such approaches, how predictions based on extrapolation from laboratory data relate to field data, and highlight where further development in EQS derivation would be welcomed. For example, can we use the relationship between chemical pressure and impact provided by an SDD to manage water quality more effectively, and is there a role for ecosystem services thinking when we derive standards for chemicals?

It is important to recognize that deriving the numerical value for a standard (the concentration) is only part of the story. Often, we focus on the derivation of the EQS, but the way a standard is implemented by regulatory agencies, such as the design of monitoring regimes, is also very important in determining the level of protection that is actually achieved. Although not specific to standards derived using an SSD, problems of implementation are often overlooked by academics and researchers since it has not prevented the setting of the standard. At the same time, regulators may be forced to make serious compromises when implementing an EQS that could be avoided through better engagement with the scientific community.

Paul Whitehouse

A botanist by training, my career has focused on researching and regulating the effects of chemicals on biological systems. My early career was with Shell Research Ltd in the UK where I undertook research into the discovery of new herbicides and pesticides. My involvement in environmental protection began in 1990 when I joined WRc, moving to my present position in the Environment Agency in 2004. I have worked in chemical hazard and risk assessment for 20 years, specializing in the derivation and implementation of Environmental Quality Standards (EQSs) for toxic chemicals and radionuclides in water and soil. These thresholds are intended to protect wildlife and human health from the toxic effects of chemicals.

My current role is to provide the technical support to meet the requirements of environmental legislation and other initiatives aimed at protecting or improving the environment. I lead the technical development of EQSs in the UK and provide technical support to the UK government in negotiations on the introduction of EQS for Priority Substances under the Water Framework Directive. I am also involved in numerous European working groups on the development and implementation of environmental standards. Between 2008 and 2011, I led a group responsible for developing European technical guidance on the derivation of EQSs for chemicals, which is now regarded as definitive guidance on the subject for the Water Framework Directive.

Current interests include the development and implementation of bioavailability-based standards for trace metals, and the implementation of biota standards for assessing risks from bioaccumulative substances in the environment.

My personal interests include gardening, cookery, and I am recent convert to fly fishing, having outwitted my first rainbow trout this Autumn.

Regulatory use of SSDs in Australia and New Zealand

Michael Warne
DSITIA Science Delivery, Australia

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Australia and New Zealand, along with many other countries, use risk-based approaches to manage and regulate chemicals in the environment. A key component of the risk approach has been the use of species sensitivity distribution (SSD) methods. SSDs are central to the Australian and New Zealand approach to managing the quality of various environmental compartments (water, sediment and soil), of additives to soils (biosolids and mineral fertilisers) an in conducting environmental risk assessments. Australia and New Zealand developed a new SSD method called BurrliOZ (http://www.csiro.au/Outcomes/Environment/Australian-Landscapes/BurrliOZ.aspx) that uses selects the distribution from the Burr Type III family of statistical distributions that best fits the sensitivity data. This method can therefore provide a good fit to many more datasets than can SSD methods that use a single statistical distribution. The Australian and New Zealand Guidelines for Fresh and Marine Water Quality (http://www.environment.gov.au/resource/australian-and-new-zealand-guidelines-fresh-and-marine-water-quality-volume-1-guidelines) were released in 2000 and are currently undergoing a review. This is examining the framework used to derive the guidelines (called trigger values). Key recommendations arising from the review are: increasing the types and sources of data that can be used; working with industry to permit the use of commercial-in-confidence toxicity data; increasing data requirements; improving the software used to calculate trigger values; increasing the rigour of site-specific trigger values; improving the method for assessing the reliability of the trigger values; providing guidance of measures of toxicity and toxicological endpoints that may, in the near future, be appropriate for trigger value derivation. A new set of sediment quality guidelines and new trigger values for a number of existing metals will be derived. In addition, trigger values for a range of organic chemicals focussing on pesticides, pharmaceuticals and personal care products will be derived. Finally, a weight of evidence approach is being included into the guidelines. These changes will improve the number and quality of the trigger values that can be derived and will increase end-users' ability to understand and implement the Guidelines in a scientifically rigorous manner.

The water quality guidelines are generic - a single value that applies to all waterways. The only exception being the trigger values of some metals that can be modified using hardness algorithms. In contrast, the Australian guidelines for contaminants in contaminated soils and in biosolids, are wherever possible, soil-specific. That is, a matrix of guidelines are generated for each contaminant depending on the values of various soil physicochemical properties known to modify toxicity. This presentation will discuss the ways that SSDs are used in Australia and New Zealand and the proposed changes arising from the current review of the Australian and New Zealand water quality guidelines.

Michael Warne

Michael is currently the Science Leader of the Water Quality and Investigation in the Queensland Department of Science, Information Technology, Innovation and the Arts. Prior to this he was a Principal Scientist at CSIRO and has held positions in the New South Wales EPA and the Universities of Queensland and Griffith University. Michael has conducted extensive research on the impacts of individual metal and organic contaminants and mixtures in terrestrial and aquatic ecosystems. He has worked extensively integrating the results of ecotoxicology into regulatory tools for managing chemicals in the environment – particularly the development of environmental quality guidelines. He was a key scientist in the development of the current Australian and New Zealand water quality guidelines and led national programs that developed contaminant guidelines for biosolids, mineral fertilisers and contaminated sites. He is participating in the current review of the Australian and New Zealand water quality guidelines. He has been awarded six outstanding performance awards and nominated for a Queensland Government Public Service Medal. Michael has been awarded over $8 million in research grants and published two editions of a book, six book chapters, 90 publications in scientific journals, eight Australian national guidelines for the environmental management of chemicals, and over 150 conference proceedings and client reports.

Use of SSD in China

Fengchang Wu
Chinese Research Academy of Environmental Sciences, China

Species sensitivity distributions (SSDs) are usually used in the development of water quality criteria (WQC) and require a large number of toxicity values to define a hazard level to protect the majority of species. In the present study, we introduced the specific use of SSD in the study of water quality criteria in China. As case studies, WQC for representative water-body pollutants in China using SSD were conducted. i.e., toxicological data for zinc (Zn), cadmium (Cd), hexavalent chromium (Cr (VI)), benzene, and nitrobenzene were collected from various databases, publications and experimental test data. And then these toxicological data were screened and then constructed into SSD curves. Then WQC for protection of the freshwater aquatic life in China against five representative pollutants were derived. The values derived in this study were compared with those issued by the US Environmental Protection Agency and the Chinese national environmental standard for surface water to identify factors underlying the differences. The results showed that the SSD curves for the five pollutants differed significantly, with the examined aquatic species being generally more sensitive to Zn, Cd, and Cr (VI) than benzene and nitrobenzene.

While SSDs based on measured toxicity values can provide a strong level of confidence for environmental protection, there is still some uncertainty in their applicability for untested species. Additionally, SSD development has been limited to a relatively few chemicals because of the requirement for toxicity data for a broad diversity of taxa. Interspecies correlation estimations (ICE) models may provide great assistance for addressing the development of WQC that are protective of species that cannot be tested. To address this need, we also tried to use ICE-based SSD in deriving WQC for zinc in China. Taken zinc for example, ICE-based-SSDs were generated using three surrogate species (common carp (*Cyprinus carpio), rainbow trout (Oncorhynchus mykiss), and Daphnia magna*) and compared with the measured-based SSD and corresponding HC5. The results showed that no significant differences were observed between the ICE- and the measured-based SSDs and HC5s. Given the similarity of SSD and HC5s for zinc, the use of ICE to derive potential water quality criteria for diverse chemicals in China is proposed. Further, a combination of measured and ICE-derived data will prove useful for assessing water quality and chemical risks in the near future. Above all, the comparative study of SSD in WQC studies may offer guideline values for future WQC studies for China.

Fengchang Wu

Dr. Fengchang Wu is currently professor and deputy General Director, Chinese Research Academy of Environmental Sciences, Ministry of Environmental Protection of China.

- 2010-present: Professor, Director of State Key Laboratory of Environmental Criteria and Risk Assessment, Chinese Research Academy of Environmental Sciences, Beijing, China
- 2007-present: Professor and director, State Environmental Protection Key Laboratory of Lake Pollution Control, Chinese Research Academy of Environmental Sciences, Beijing, China
- 2004-2008: Professor, and deputy director, State Key Laboratory of Environmental Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China

Expertise

Water quality pollution mechanism and process
Environmental criteria and risk assessment
Environmental pollution control technology and management research

Recent contributions and initiatives

Chief Scientist, National Key Basic Research Project (973 project) “Key Lake Environmental Quality Changes and Water Quality Criteria in China” (No: 2002CB418200), 2007-2012.
Chief Scientist, Key Project of Environmental Ministry of China “preliminary investigation of Environmental Criteria in China”, 2009-2011

Overview of publications and awards publications

Over 160 peer-review papers
6 books (in Chinese and in English)
Over 50 presentations worldwide

Awards

- New Century 100-1000-10000 Talents Programt” (National levels)
- Excellent Young Science and Technology Award, China Government, 2006
- National Excellent Young Scientist Fellowship, Natural Science Foundation of China (NSF), 2005
- ESTANSGP Best article Award, Excellent Science and Technology Articles in Natural Sciences in Guizhou Province (ESTANSGP), 2006
- STAGP Best Award, Science and Technology Award in Guizhou Province (STAGP)
- 2004 Hou DeFeng Young Scientist Award, Chinese Association of Mineral, Petrology and Geochemistry, 2004
- Excellence Award of “One-hundred Scientist Program”, Chinese Academy of Sciences, 2004
- “One-hundred Scientist Program” Fellowship, Chinese Academy of Sciences
- Excellence Award for Ph.D. Graduate, Institute of Geochemistry
- Award for “The state environmental protection science and technology “ first prize,2012
- Award for “National science and technology progress prize” second prize, 2013

Use of SSD to derive no-effect thresholds for water quality guidelines and ecological risk assessments in Canada

Anne Gosselin
Environment, Canada

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In Canada, species sensitivity distributions (SSDs) are used to derive “no effect” thresholds that serve to determine water quality guidelines for aquatic life as well as Predicted-No-Effect-Concentrations (PNECs) in ecological risk assessments of chemicals. The Federal Water Quality Guidelines (FWQGs) are developed to meet the needs of risk assessment and risk management of chemicals under the Canadian Environmental Protection Act, 1999 (CEPA 1999). In addition, Canadian WQGs are developed under the auspices of the Canadian Council of Ministers of the Environment (CCME) based on priorities identified by federal, provincial and territorial jurisdictions. Moreover, under CEPA 1999, regulatory ecological and human health risk assessments are conducted for substances identified as priorities on Canada’s Domestic Substances List.

190BThe FWQGs, CCME guidelines and PNECs used in ecological risk assessments all identify thresholds for aquatic ecosystems that are intended to protect all forms of aquatic life and all life stages for indefinite exposure periods. The methodology used to derive these thresholds is the “Protocol for the Derivation of Water Quality Guidelines for the Protection of Aquatic Life” (CCME 2007). SSD is the preferred approach for FWQGs, CCME guidelines and PNECs. It follows these steps: toxicity data collection, evaluation and selection, SSD plotting, verification of statistical assumptions including determination of the goodness-of-fit (i.e., selection of the model), and determination of the FWQG, CCME guideline and/or PNEC. They are set at the 5th percentile of the SSD, which may, in the case of the PNEC used for risk assessment, be divided by an assessment factor if deemed necessary.

191BExamples of the use of SSDs in Canada will be presented, including the federal water quality guidelines and risk assessment for metals (vanadium and cobalt) and the antimicrobial triclosan.

Anne Gosselin

Ms. Anne Gosselin is a Senior Evaluator in the Ecological Assessment Division of Environment Canada. She has been in this position for the last six years conducting ecological risk assessments of chemicals under Canada's Chemicals Management Plan. She specializes in the assessment of metals. From 2004 to 2007, Ms. Gosselin was working as an evaluation officer at the Pest Management Regulatory Agency of Health Canada where she conducted risk assessments of pesticides. She started her career as a research project manager working with the Quebec Ministry of the Environment on a project pertaining to the toxicity of industrial wastes. Ms. Gosselin holds a M.Sc. degree in Water Sciences from INRS – University of Quebec, and a B.Sc. degree in Biology from Laval University. In her current position at Environment Canada, she has led preparation of a number ecological assessment reports, covering a range of substances, notably leading on metals related issues.

Use of SSDs in the USA – endangered species and water quality criteria

Mace Barron
Environmental Protection Agency, USA

Species sensitivity distributions (SSDs) are used in the United States (US) in the development of national ambient water quality criteria (AWQC), with site-specific and numeric modifications to protect sensitive taxa including threatened and endangered species. The US Environmental Protection Agency (EPA) first used SSDs constructed of acute toxicity values in 1978, with formal guidance issued in 1985 for computing 5th percentile hazard concentrations (HC5) from SSDs constructed of at least eight families with acceptable toxicity data. Additional minimum data requirements (MDRs) include acceptance of only North American species and specific taxa diversity requirements that have limited the development of AWQC to only 47 chemicals. EPA is currently considering alternative approaches for developing SSD-based AWQC, with the recognition that species composition appears to affect HC5 estimates for aquatic species more than differences in geography or habitat of the assemblage. The protectiveness of SSD hazard concentrations used in endangered species risk assessment remains a concern because of uncertainty in sensitivity compared to standard test species. In a recent study, the relative sensitivities of US federally listed and non-listed aquatic species were compared for a broad range of chemicals. The SSD HC5s and HC1s were lower than 97 and 99.5% of all endangered species mean acute LC50s, indicating that the use of SSDs as distribution-based risk assessment and criteria development approaches can be generally protective of listed species. A recent US National Academy of Sciences report suggested SSDs should be applied in endangered species risk assessments as an alternative to general uncertainty factors. This presentation will overview US applications of SSDs in AWQC development and listed species assessment, and include perspectives on modifying MDRs and adopting new approaches to meet taxa diversity requirements.

Mace Barron

Dr. Mace G. Barron is Acting Associate Director of Science at the EPA Gulf Ecology Division, in Gulf Breeze, Florida, USA. Mace has worked in EPA's Office of Research and Development for 10 years and directed ecological effects research and model development to predict risks to endangered species, reef building corals, and marine fish populations. He received his B.S. and M.S. degrees in Fisheries Science, a PhD in Pharmacology/Toxicology, and conducted post-doctoral research on chemical bioaccumulation and biotransformation in crustaceans and fish. He has over 25 years of work experience, including senior scientist positions in the chemical industry and in firms performing Natural Resource Damage assessments. He has published over 100 peer reviewed journal articles and book chapters on chemical bioaccumulation, ecological risk assessment, photo enhanced toxicity, toxicity estimation and species sensitivity distributions (SSD). Mace is co-developer of EPA's Web-ICE toxicity estimation tool, and has published extensively on the technical basis of interspecies toxicity extrapolation and SSD development. Currently Mace is a member of the US EPA Risk Assessment Forum and effects lead for the EPA team developing approaches for applying computational chemistry to aquatic toxicity mode of action assignment and QSAR model development.

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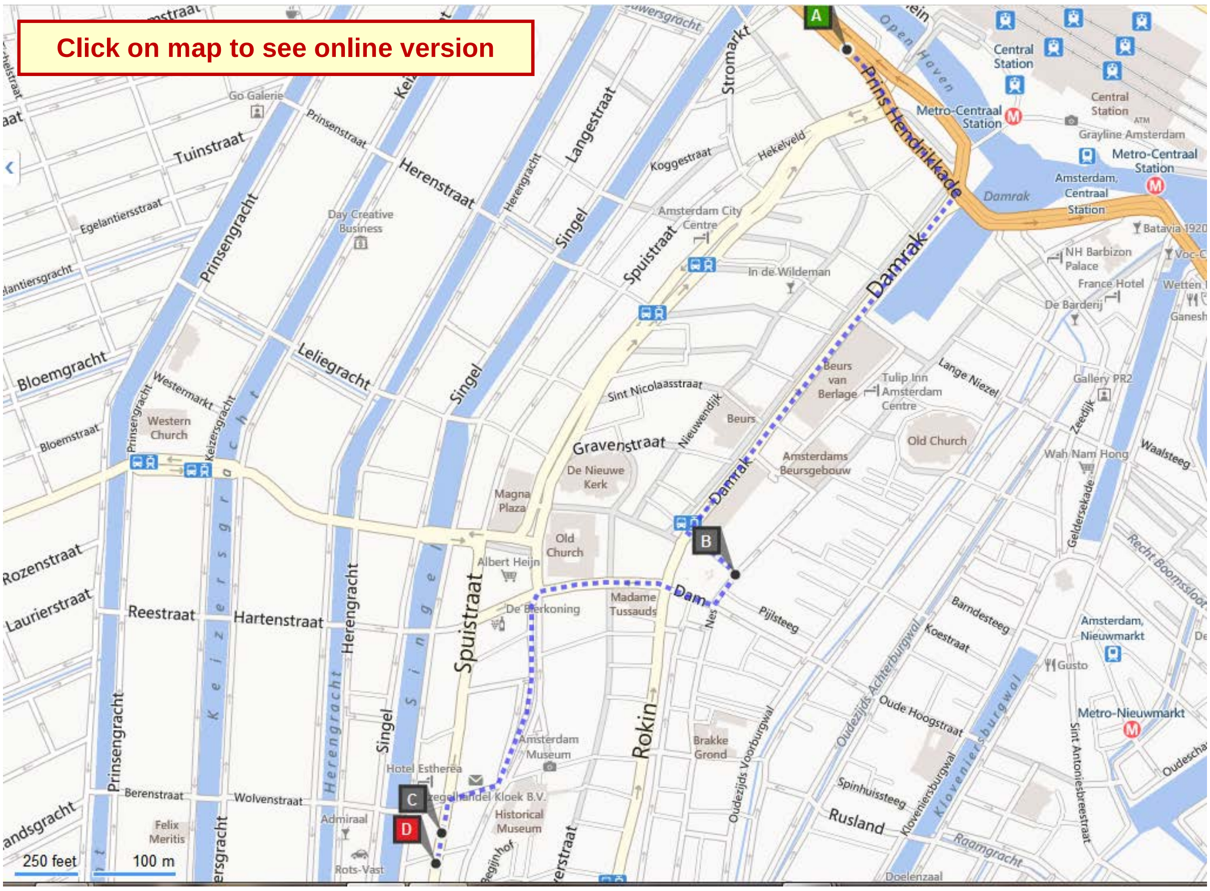
LOGISTICS

VENUE

NH Grand Hotel Krasnapolsky
Dam 9, 1012 JS Amsterdam (The Netherlands). Tel. +31.20.5549111
(***B** on the map below, a 0.8 km 10 minute walk from the Central Station – A on the map*)



The NH Grand Hotel Krasnapolsky hotel in Amsterdam is located in the very heart of the city, right on the central Dam square near many major tourist and business attractions. If you arrive by car, the hotel has a parking attendant at your service and a secure paid garage. There are bus and tram stops right outside the hotel. The central train station is only 5 minutes away by public transport and Schiphol Amsterdam Airport is just a 25 minute taxi or car ride.

The restaurant for the evening of 11 February is a 0.6km 8 minute walk from the hotel (**C** on the map): Restaurant Haesje Claes, Spuistraat 273-275, Amsterdam, Tel.+31 20 624 9998

The restaurant for the evening of 12 February is also a 0.6km 8 minute walk from the hotel (**D** on the map): Restaurant D'Vijff Vlieghen, Spuistraat 294-302, Amsterdam, Tel.+31 20 530 4060

REGISTRATION AND ENQUIRIES

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