

New tool for identification of chemicals with high risk potential

Researchers at NERI in Denmark have, as part of their contribution to the EU-funded project NoMiracle, developed a method to rank substances such as pesticides and biocides with respect to different criteria of toxicity and exposure. Now it is possible for instance to identify the most hazardous chemical or the five most hazardous chemicals in defined scenarios. This is important when

the community prioritises its administration of hazardous chemicals. The new method will help ensure that chemicals are considered systematically and effectively with respect to potential harmfulness to human health and eco-systems. The tool will take into account variables like scenario conditions and potential health effects.

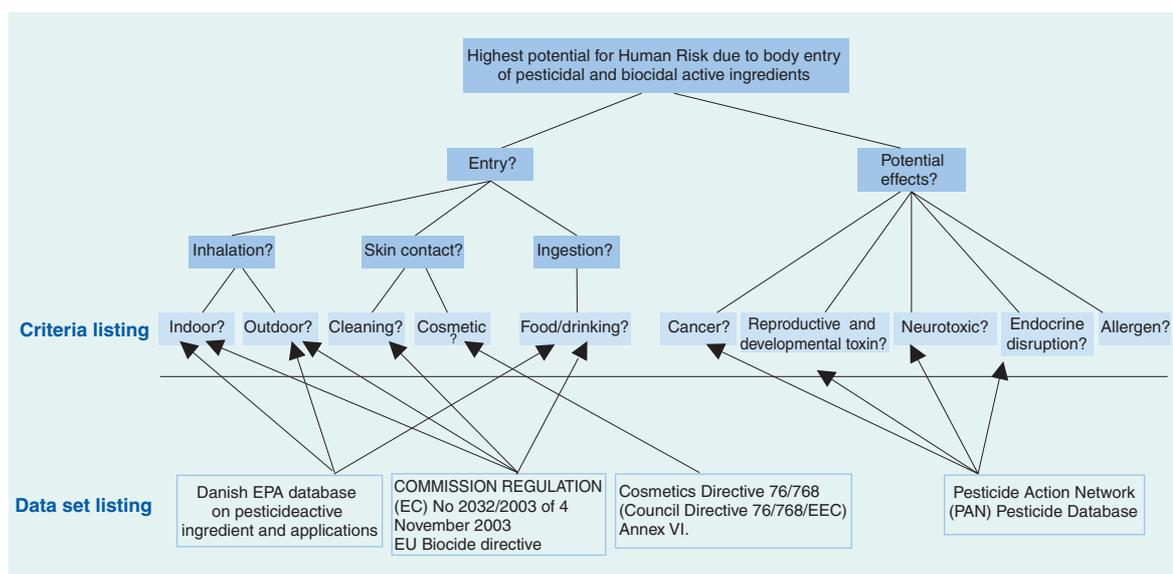


Figure 1.

Derivation of criteria and relation to existing data sets. The list of criteria are derived using a top-down procedure where factors are subdivided into sub-factors. The most detailed sub-factors form the criteria set. Below the line are listed data sets that are used for quantification (ranking) for the criteria and thus as descriptors during the sub-sequential multi-criteria ranking.

In this edition

1. New tool for identification of chemicals with high risk potential
5. First open international NoMiracle workshop, Ispra, Italy, June 8-9, 2006
6. First year of NoMiracle
7. NoMiracle at SETAC Europa in den Haag
7. Limits of endocrine disrupters in terms of mixtures; the ACE project
8. Mixture Toxicity Workshop in Krakow Poland April 3 - 6, 2006, Only open for invited scientists
8. NoMiracle co-ordination

The NoMiracle Newsletter visited NERI researchers

Peter Borgen Sørensen and Marianne Thomsen who developed the tool

Can you describe the idea behind this tool?

As it often happens good ideas come from the identification of problems. Here the problem was to prioritise between the numerous chemicals that surround us in our households. A lot of effort is put into the development of more advanced risk assessment methods but the efficiency of these methods is lost if they are not applied to solving the most relevant problems. So the new tool lets us make a pre-selection of problems prior to risk assessment. We do not assess risk, but only demonstrate that one situation is more risky than another one, thereby producing a risk ranking.

But don't we already know how to rank chemical risks? What steps do you propose?

It is not a straightforward process to rank risks because many factors must be taken into account. The challenge is to take a multi-criteria decision. The first step is to define a good set of criteria and this is not a trivial task. The selected criteria will naturally control the possible outcome of the scenario ranking process. Therefore, our work includes developing a paradigm for criteria selection, in which expert knowledge is used in a systematic way such that a criterion reflects the best possible state of knowledge. It may be the case that a criterion is derived but no data exist to describe the criterion. In such cases a data gap exists that must be addressed in future research activities. The NoMiracle tool therefore highlights what needs to be learned in order to arrive at an even more reliable ranking.

The second step is to feed the data that describe the criteria for each substance into a ranking procedure. Here the challenge is due to missing knowledge about how important every single criterion is for the task of identifying the risk level. We have therefore developed a statistical method to help address the uncertainty that remains when we have chosen criteria in step one. The precautionary principle tells us to take into account

all ranking outcomes that may be possible and not just focus on the most possible outcome. If the precautionary principle is ignored in the work of singling out the most relevant problems to which assessment resources should be assigned, then this principle is violated in the entire risk assessment because it may focus on the wrong problem. The statistical calculation in our new selection procedure takes into account all possible risk ranking results. In this way it is possible to estimate that if e.g. 10 chemicals are ranked as high priority for risk assessment out of a total of 100, then there is a 95% chance that our set of substances includes the one that will show highest risk. In this way we can define how cautious we wish to be.

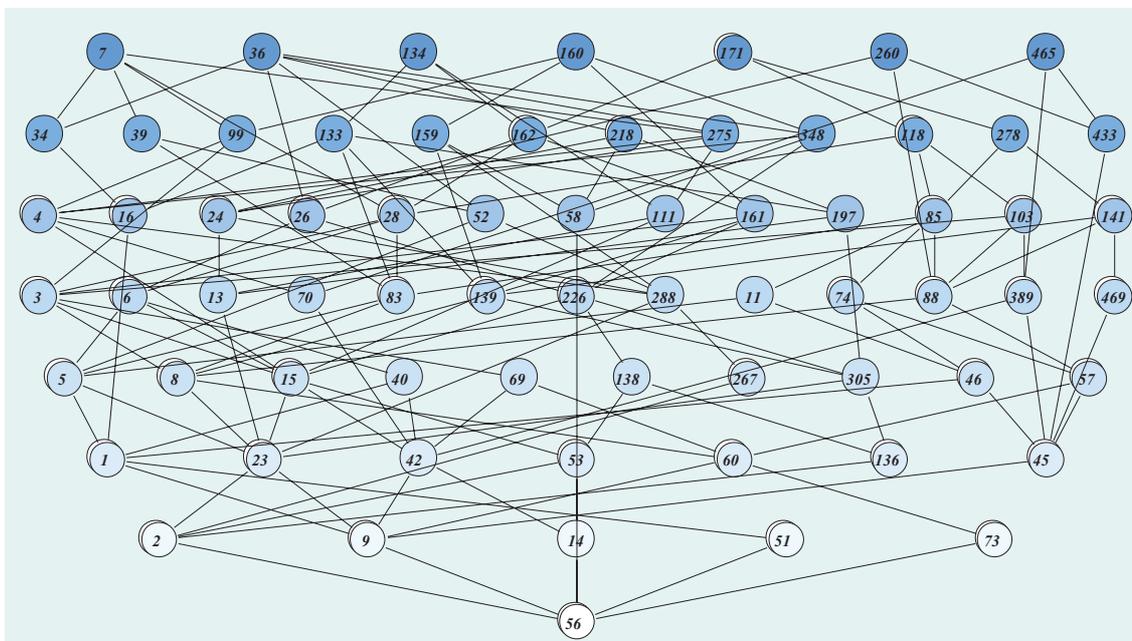
Can you give an example of applying the method?

The first test application of the method has been performed on a set of 582 household pesticides and biocides. The diagram below shows how the criteria are derived and related to data sets. Figure 1 corresponds to step one of our procedure. It shows 9 criteria derived in order to rank the household chemicals. Each criterion is described by data assembled in databases and/or regulations.

Figure 2 then shows the next step in which data for each criterion are fed into a ranking procedure called Partial Order. The 9 criteria are used simultaneously. The number labels correspond to specific active ingredients. Some of the pesticides/biocides are equal on all nine criteria and are thus positioned in the exact same position in the Hasse diagram. In that case the Hasse diagram only shows one ID label in a double circle. For instance, the ID 171 has the same criteria values as at least one more ID that is not made visible. In the Hasse Diagram, a rank is assigned between two pesticides only if no conflicts exist in the rank among all the criteria, i.e. when no criterion disagrees on ranking one chemical above or below another.

Figure 2. Hasse Diagram for the 582 household pesticides and biocides using nine criteria.

The diagram is drawn using the software WHasse, Brüggemann et al, 1999.



The Hasse diagram in Figure 2 shows 7 top candidates that all potentially are worst case substances. Our newly developed method can make a more detailed differentiation between the chemicals as shown in Figure 2.

***How about information on chemicals?
Is the information available sufficient to run the model or must more data be generated?***

There are many available data sets of different quality, but a data gap is often seen when it comes time to describe the criteria. This is the reason why our top-down approach in step one, as shown in Figure 1, is important. Otherwise the criteria setting itself will often be biased by the existence of available data sets, and thus suppress the criteria that are not described by available data but which may be important.

Criteria can obviously be of very different nature, could you define "criterion"?

There is no single definition of "criterion". What is important is to make a clear definition in order not to be confused in the application of criteria. In this work the criteria are defined as factors that must be addressed in the selection process.

This definition helps to structure the selection in a highly efficient way. The criteria become theoretically-based and a data set can be evaluated by considering: (1) How well does the data set describe the criterion (uncertainty of analogy)? (2) What is the data variability (uncertainty of data value)?

How do you decide whether a criterion should be included or not, and how does it affect the results?

It is a key issue to decide which criterion to include. That has to be done based on expert knowledge. A wrong selection of criteria will yield a faulty result; the statement "garbage in, garbage out" holds here. About 10 criteria can be handled by the existing method so that sets an upper limit. However, it is easy to perform a sensitivity analysis by comparing the results from different combinations of criteria sets.

NoMiracle Newsletter No. 2

NOvel Methods for Integrated Risk Assessment of Cumulative stressors in Europe

Did you experience problems in the development of the tool?

The selection of problems for detailed risk assessment will never be perfect; it will always be based on some set of assumptions. The challenge is to minimise the impact from these assumptions on the selection. The method that is used assumes that the criteria can be well described as only "high/low", which is a limitation in relation to categorical and continuous data sets. The level of detail in the criteria value setting may be improved if there is time for recursive steps. However, test cases using several criteria show that the uncertainty in the entire selection procedure becomes so high that the overall benefit gained from a more detailed value setting of the single criterion is limited.

Who or what will benefit from the tool?

The tool is firstly developed to help identify the highest priority problem for detailed risk assessment and thus will support the work done by other researchers in NoMiracle. In this way, we will be passing our results along to NoMiracle Work Packages dealing with risk assessment (Research Pillar 4). We have held a workshop with this Pillar to assure integration. In general the method is useful in many aspects of prioritising and thus relevant for identifying hot spots for more detailed examination of environmental and human health impacts. The NoMiracle software we have developed will thus also be of value for EU or national regulators and administrators.

When will the method be ready to use in European or national administration of chemicals?

The method will become available during year 2006.

Will this influence the potential application of the precautionary principle?

Yes, our tool will allow the precautionary principle to be better implemented in the legislation, through supporting the identification of missing knowledge and quantifying the impact from missing knowledge on the background for risk assessment. Better handling of missing knowledge is a condition for efficient use of the precautionary principle.

For more information contact:



Peter
Borgen Sørensen:
pbs@dmu.dk



Marianne
Thomsen
mth@dmu.dk

Reference

Brüggemann, R., Bücherl, C., Pudenz, S., Steinberg, C.E.W., (1999), Application of concept of partial order on comparing evaluation of environmental chemicals, Acta Hydrochim, Hydrobiol, 27, 170-178.

Open international workshop on:

Ecological and Human Health Risk Assessment:

Focussing complex risk assessment and identification of highest risk conditions in:

Ispra, Italy , June 8-9 2006

NoMiracle Newsletter No. 2

NOvel Methods for Integrated Risk Assessment of CumuLative stressors in Europe

In the context of the project

NoMiracle :

Novel Methods for Integrated Risk Assessment of Cumulative Stressors in Europe

The aim of the workshop is to discuss the main outcomes of the Project concerning criteria for the selection of risk scenarios, mapping and visualizing risk, and communicating it to the general public, the decision makers and scholars in other disciplines.

During the workshop, a series of communications by the Project participants will illustrate the main topics and will introduce discussion among the participants.

Discussion sessions will allow non-project participants to present experiences and research related to the workshop topics.

All contributions will be made available through Workshop proceedings in electronic format via www.

Main Topics:

- Scenario screening to support risk assessment
- Geographical risk mapping
- Communication of methods to users: presentation of experiences in mapping of human health risks;
- Highlighting the potential implications for application of the precautionary principle.

Target groups of participants:

- Scientists: GIS mapping, Eco-system, Human health, Eco-toxicity, Risk assessment and management
- Decision makers at a technical level
- Industry
- SME's
- NGO's
- International organisations

Scientific Committee:

Matthieu Craye, Jack Faber, Patrik Fauser, Silvio Funtowicz, Mikael Hilden, Trine Jensen, Joost Lahr, Bernd Munier, David Pennington, Alberto Pistocchi, Ad Ragas, Suresh Rastogi, Uwe Schlink, David Spurgeon, Peter Sørensen, Marianne Thomsen, Marco Vighi

Organisation:

EC-Joint Research Centre, Soil and Waste Unit, ENSURE Action 2131.

Alberto Pistocchi Alberto.Pistocchi@jrc.it

Ph. +390332785591 - Fax +390332785601

Via E.Fermi, 1 - 21020 Ispra (VA), Italy

For more information and program in full see:

NoMiracle web page: <http://nomiracle.jrc.it>

First year of NoMiracle

The first year of the Integrated Project NoMiracle ended the 31 of October 2005 and the Consortium is now facing the evaluation of its first annual report to the Commission. Another challenge this first year has been to ensure the communication within the project. Major steps to meet this challenge has been the kick off meeting in Barcelona, January 2005, meetings of The NoMiracle Management Board, The NoMiracle General Assembly and The NoMiracle Advisory Board as well as Research Pillar meetings, The NoMiracle Internet and Intranet homepages. On top of this is an immense load of communication by email and telephone.

A vast amount of scientific work has been initiated to fulfil the seven major objectives of NoMiracle (see Box). The four Research Pillars in NoMiracle has so far delivered 12 reports and scientific manuscripts. Those publicly available can be downloaded from the NoMiracle Internet homepage. <http://nomiracle.jrc.it>

The seven major objectives of NoMiracle

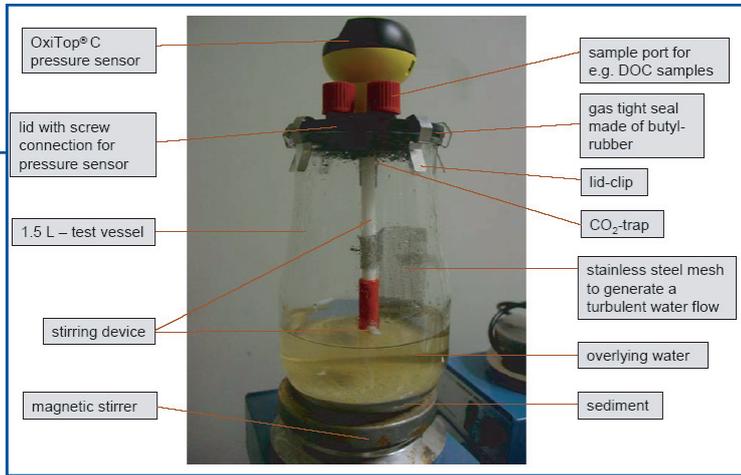
1. To develop new methods for assessing the cumulative risks from combined exposures to several stressors including mixtures of chemical and physical/biological agents
2. To achieve more effective integration of the risk analysis of environmental and human health effects
3. To improve our understanding of complex exposure situations and develop adequate tools for sound exposure assessment
4. To develop a research framework for the description and interpretation of cumulative exposure and effect
5. To quantify, characterise and reduce uncertainty in current risk assessment methodologies, e.g. by improvement of the scientific basis for setting safety factors
6. To develop assessment methods which take into account geographical, ecological, social and cultural differences in risk concepts and risk perceptions across Europe
7. To improve the provisions for the application of the precautionary principle and to promote its operational integration with evidence-based assessment methodologies

Work performed and results achieved

During the first 12 months the project has promoted strong interactions among interdisciplinary research lines. According to the plan, activities were started successively.

The major activity has been to develop the data background for scenario selection, exposure assessments, uncertainty assessments and risk mapping. Also problems with data gaps and uncertainty related to data values and estimation have been dealt with. Procedures are under development which can be included in a systemic way based on a paradigm for criteria setting.

In the area of computer science and data base management the concept of ontology based knowledge is investigated for adoption into a hierarchical criteria development principle. A paper on resources and uncertainties in evaluation of chemicals is published (Sørensen et al., 2005). The focus is on a methodological implementation of precaution into the screening phase. This development is further supported by a paper on a new paradigm for multi-criteria ranking developed for supporting risk assessment is ready for submission.



New water-sediment test system developed in NoMiracle.

Preliminary results from a state-of-the-art overview on cumulative risk mapping shows that a lot has been done on mapping of pollution, pollution sources and environmental risks of single pollutants, but that mapping cumulative or integrated risks seems to be a new area with very little done to this date. An ongoing study on aggregation of spatial data demonstrates the potential impact of different aggregation methods on risk maps.

A review has been produced of scientific literature on the integration of human and ecological risk assessment, and of the origin and development of assessment factors in human and ecological effect assessment. Motives for integration and different types of integration are identified and discussed.

Human and ecological assessment factors are compared, and similarities and differences identified. Options to further harmonize human and ecological extrapolation procedures have been identified.

A new water-sediment test system for chemicals has been developed. The design of the new test system is close to the OECD Guideline 301 C (MITI I). The obtained results showed that the developed water-sediment test system can be considered as ready for use for the generation of biodegradation kinetics within NoMiracle.

In order to develop new methods for assessing the cumulative risks from combined exposures to several stressors including mixtures of chemical and physical/biological agents, work has been initiated on two existing mixture toxicity models for binary and more complex chemical combinations. A guidance document and simple software program to be used for the experimental design and data analysis of mixture toxicity experiments has been produced. A series of partners are undertaking the essential initial single compound and then mixture tests in a diversity of taxa (ranging from single celled eukaryotes to in vitro human cell line systems).

Sørensen, P.B., Lerche, D.B. & Brüggemann, R. (2005): Resources and uncertainties in evaluation of chemicals: basic methodological developments. - Water Science & Technology 52(6): 235-242.

NoMiracle Newsletter No. 2

NOvel Methods for Integrated Risk Assessment of Cumulative stressors in Europe

NoMiracle at SETAC Europe in the Haque May 7 - 11, 2006

The NoMiracle partners present a long series of platform and poster presentations. Some of the NoMiracle participants have been active in organising the conference, and others will act as chairs or co-chairs. The NoMiracle related presentations will be announced on the Homepage (www.nomiracle.jrc.it).

Limits of endocrine disrupters in terms of mixtures; the ACE project

The new issue of the CREDO Newsletter includes an article on the ACE project that was concluded in 2005. Knowledge on limits for multi-component mixtures of endocrine disrupting compounds was very limited prior to the ACE project. The primary objective of ACE was to contribute to the hazard assessment of EDCs in the aquatic environment. For more information see the CREDO Newsletter:

<http://www.credocluster.info/docs/newsletter/credonews5.pdf>

Workshop on mixture toxicity for invited experts

The Society for Environmental Toxicology and Chemistry (SETAC) and the EU Integrated Project NoMiracle are organising a workshop on mixture toxicity. Leading researchers have been invited to a meeting in Krakow from April 3 to 6 to discuss the state of the art of mixture toxicity research and its use in environmental and human health risk assessment. They represent leading governmental and private institutions as well as authorities in charge of chemicals regulation.

The aim of the workshop is to discuss the state of the art of mixture toxicity research, in the fields of human health and ecotoxicology, and its use in risk assessment. Final aim is a book that provides an overview of the steps, in form of a "decision tree" with chapter references, to be taken when performing the risk assessment for a certain combination of chemicals (mixture) and a certain organism (human, animal, plant etc). This should take into account exposure pathways, routes of uptake, uptake kinetics, metabolism, modes of action etc. These processes can be organism-specific and also chemical-specific.

Workshop Setup

After a brief introduction, addressing the background and aims of the workshop, and two lectures dealing with risk assessment and highlighting the approaches and research needs from a human health and an ecotoxicological perspective, respectively, the workshop will be held around five topics; *Bioavailability and exposure, Kinetics, Mechanistics, Test design, data evaluation and mixture characterization and Risk assessment*



NoMiracle co-ordination

Visit NoMiracle at:
<http://www.nomiracle.jrc.it>

For further information contact

NoMiracle Secretariat
E-mail: nomiracle@dmu.dk

- Project co-ordinator: Dr. Hans Løkke, National Environmental Research Institute, Vejlshøvej 25, P.O. Box 314, DK-8600 Silkeborg Denmark
Phone +45 8920 1482, Fax +45 8920 1414
E-mail: hlo@dmu.dk
- Databases and selection of scenarios: Dr. Hanne Bach, National Environmental Research Institute, Denmark
E-mail: hba@dmu.dk
- Exposure assessment: Professor Gerrit Schüürmann, UFZ, Umweltforschungszentrum Leipzig, Germany
E-mail: gerrit.schuurmann@ufz.de
- Effects assessment: Dr. Dave Spurgeon, NERC, Centre for Ecology and Hydrology, United Kingdom
E-mail: dasp@ceh.ac.uk
- Risk Assessment: Dr. Ad Ragas, Radboud Universiteit Nijmegen, The Netherlands.
E-mail: A.Ragas@science.ru.nl

Subscription on NoMiracle Newsletter:
send an e-mail to Nomiracle@dmu.dk

The integrated project NoMiracle is funded by the European Commissions Sixth Framework Programme.

EC Scientific Officer for the project:
Dr. Jürgen Büsing.