iEMSs 2008: International Congress on Environmental Modelling and Software
Integrating Sciences and Information Technology for Environmental Assessment and Decision Making
4th Biennial Meeting of iEMSs, http://www.iemss.org/iemss2008/index.php?n=Main.Proceedings
M. Sànchez-Marrè, J. Béjar, J. Comas, A. Rizzoli and G. Guariso (Eds.)
International Environmental Modelling and Software Society (iEMSs), 2008

Environmental Protection, Sustainable Development & Risk Management with Emphasis on Environmental Chemicals

Kristina Voigt
Helmholtz Zentrum, Muenchen, German Research Center for Environmental Health, Ingolstaedter Landstr. 1, 85764 Neuherberg, e-mail: kvoigt@helmholtz-muenchen.de

***Keywords**: Environmental risk, environmental risk assessment, environmental risk management, sustainability, sustainable chemistry, green chemistry, environmental models, environmental decision support systems, Hasse Diagram Technique*

The relevance and acceptance of **environmental protection** in society has been changing over the past decades. According to my own experience in Germany the topic was of high importance at the end of the seventieth till mid 1980ieth. Then the interest turned to other important societal subjects such as risk of unemployment, retirement pay, reunification, warlike operations etc. These days a lot of environmental research is performed in the direction of human health and the environment. Currently another focus lies on the issues regarding climate change. Furthermore the subjects energy and the environment receive more attention.

Only recently the terms environmental protection often in connection with **sustainability** and **sustainable development** receive an increasing interest. **Sustainability** is a characteristic of a process or state that can be maintained at a certain level indefinitely. The term, in its environmental usage, refers to the potential longevity of vital human ecological support systems, such as the planet's climatic system, systems of agriculture, industry, forestry, and fisheries, systems on which they depend in balance with the impacts of our unsustainable or sustainable design (WIKIPEDIA, 2008). **Sustainable development** is a pattern of resource use that aims to meet human needs while preserving the natural environment so that these needs can be met not only in the present, but in the indefinite future. The term was used by the Brundtland Commission which coined what has become the most often-quoted definition of sustainable development as development that "meets the needs of the present without compromising the ability of future generations to meet their own needs"(United Nations, 1987). **Sustainable development** does not focus solely on environmental issues. The United Nations 2005 World Summit Outcome Document, refers to the "interdependent and mutually reinforcing pillars" of sustainable development as economic development, social development, and environmental protection (United Nations, 2005). Concerning the chemicals' policy a stable balance between economic interests and the challenging protection of the environment and human health must be given. Only with respect to this balance we will be able to further profit from the usefulness of chemistry and chemicals, e.g. pharmaceuticals, pesticides, polymers, fertilizers, building materials, flame retardants, etc. In this context we often talk about **sustainable chemistry** or **green chemistry** (Richter, 2008). The discussion, can chemists contribute to sustainable development, and in which way is rather young. The chemical industry has achieved significant improvements with regard to the reduction of direct emissions and waste. This is a result from the high technical level which has been developed in the meantime, under consideration of the saving of energy and raw material. The most hazardous chemicals like PCBs (Polychlorinated biphenyls) and other POPs (Persistent Organic Pollutants) are banned.

Sustainability targets, however, continue to play only a subordinate role in the development of new chemicals and chemical processes. New chemicals should fulfil their function in an optimised manner; but the proportion of new chemicals which are classified as dangerous is not lower than that of existing chemicals. When developing new processes or products, criteria like low resource demand, low waste, low toxicity are mostly of minor importance. Sustainability is still waiting to become a main goal worthwhile being conquered (Steinhäuser, 2004). Today, the controversial discussion on chemicals has generated a more differentiated thinking necessary to minimize the **risks** posed by chemicals and chemical processes.

The risk decision process is traditionally divided into two stages, **risk assessment** and **risk management**. **Risk assessment** is the major bridge linking science to policy.

The European risk assessment principles for new and existing chemicals are laid down in Commission Directive 93/67/EEC and 1488/94 (European Commission, 2003), respectively. Increasing concern that these European Commission regulations do not provide sufficient protection and that less than hundred high priority substances underwent a risk assessment in the past 10 years led to a review of the current policy on chemicals. A new system called REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) has recently been adopted (European Commission, 2006). The aim of REACH is to improve the protection of human beings (comprising of workers, consumers, and humans indirectly exposed via the environment) as well as ecosystems in the aquatic (water and sediment) and terrestrial compartments (including top predators) from adverse effects of chemicals while maintaining the competitiveness and enhancing the innovative capability of the EU chemicals industry. Within the context and scope of REACH, there is a need to be able to efficiently perform risk assessments on thirty thousands chemicals manufactured in or imported into Europe.

An e**nvironmental chemical risk/safety assessment** usually proceeds in the following sequence: **hazard assessment**, **exposure assessment** and **risk characterisation**. In the **hazard assessment**, reliable and relevant longterm (chronic) ecotoxicity data for organisms belonging to different trophic levels are gathered. For a limited effects database, the predicted no effect concentration (PNEC) is calculated by applying an assessment factor (AF), reflecting sources of uncertainty, to the lowest ecotoxicity value observed. For a sufficiently large effects database, a species sensitivity distribution (SSD) can be used to derive the PNEC value. The 5th percentile is used as the PNEC estimate, after application of an AF between one and five to cover remaining uncertainties (European Commission, 2003). In the **exposure assessment**, a distinction is made between different spatial scales (European Commission, 2003). The local scale considers the vicinity of a point source and the local predicted environmental concentration (PEClocal) is calculated. The regional scale assesses the exposure levels due to diffuse/widespread releases in a larger region (PECregional). The PECregional acts as the background concentration for the local assessment. The technical principles, described in the EU TGD – Technical Guidance Document (European Commission, 2003), are implemented in the computer program EUSES (European Commission, 1998). EUSES (European Union System for the Evaluation of Substances) software first calculates releases of chemicals based on the volume produced or imported, the use pattern, and the physical-chemical properties of the chemical concerned. These release estimates are subsequently translated into PECs for each environmental compartment (air, water, sediment, soil) based on the transport and fate of the substance. The **risk characterisation** comprises of a quantitative comparison of the PEC, for most substances under REACH estimated through modelling, with the PNEC. The risk characterisation ratio (RCR), or PEC/PNEC ratio, larger or equal to one signifies that there is a potential risk of adverse effects occurring. A RCR smaller than one signifies no need for further information and/or testing and/or implementing risk management measures (RMMs) (Verdonck, 2008). Improvements and enhancements concerning the EUSES risk assessment model / software are suggested by several authors.

Jager et al. are of the opinion that probabilistic risk assessment is preferable to deterministic quotients to address the complex problems of chemical risk assessment and risk management. Nevertheless, it takes time to change the conventional and well-accepted approaches, and risk managers as well as risk assessors need to familiarise themselves with probabilistic methods and distributions of risk. Perhaps it is possible to use a deterministic and a probabilistic approach side–by-side in a decision support system. In this way, risk assessors and risk managers can compare the outcomes and get accustomed to dealing with probability distributions (Jager, 2001). A more recently published paper by Verdonck et al.

demonstrates the usefulness of an efficient risk refinement tool based on sensitivity and uncertainty analysis on the risk assessment model EUSES (Verdonck, 2008).

In **risk assessment**, scientific data on toxicological and ecotoxicological effects are used to determine possible adverse effects and the exposure levels at which these effects may be expected. These effect levels are then compared to predicted (or monitored) exposures in order to characterize the risk. The risk characterization is used as a part of the basis for risk management decisions on appropriate measures to handle the risk. Such decisions range from taking no actions at all, via limited measures to reduce the highest exposures, to extensive regulations aiming at completely eliminating the risk, for instance by prohibiting activities leading to exposure. In the **risk management** decision, factors other than the scientific assessment of the risk are taken into account, such as social and economical impacts, technical feasibility, and general social practicability. According to the European Commission Technical Guidance Document for risk assessment (European Commission, 2003) "the risk assessment process relies heavily on expert judgment". Issues to be determined by expert judgment include central issues in many risk assessments, for instance the relevance of test data obtained with non-standardized methods, the interpretation of conflicting data, data quality evaluation, assessment of carcinogenicity and mutagenicity, and whether an effect is causally connected to exposure or not (European Commission, 2003). The combined effect of scientific uncertainty and a high degree of flexibility and reliance on individual experts make it in practice impossible to achieve a risk assessment process that is fully consistent and systematic in all aspects. It is therefore essential to scrutinize and evaluate the risk assessment process, in order to learn more about (1) how scientific information is reflected in risk assessment, (2) how and to what degree risk assessment influences risk management, (3) to what degree the risk decision process as a whole satisfies general quality criteria such as efficiency, consistency, and transparency. Hansson and Ruden made an approach to evaluate the risk decision processes (Hansson, 2006).

The complex topic of environmental chemical risk assessment has hence to be seen in connection with environmental models and environmental decision support systems (EDDSs). A DSS (decision support system) has been defined in many different ways, but it can be regarded in general as an interactive, flexible, and adaptable computer based information system especially developed for supporting the recognition and solution of a complex, poorly structured or unstructured, strategic management problem for improved decision-making. It uses data and models, provides an easy, user-friendly interface, and can incorporate the decision-makers own insights. In addition, a DSS is built by an interactive process (often by end-users), supports one or more phases of decision-making, and may include a knowledge component. An environmental decision support system (EDSS) often consists of various coupled environmental models, databases and assessment tools, which are integrated under a graphical user interface (GUI), often realized by using spatial data management functionalities provided by geographical information systems (GIS). An overview of the current activities, methods and tools in this area is outlined by Matthies et al. (2007).

In my further presentation I will give an example applying a software tool for environmental decision support based on the theory of partially ordered sets. The background and application of the software tool named Hasse Diagram Technique were introduced by the author recently (Voigt, 2006). This environmental decision support tool is now applied on the ranking of environmental pollutants found in soil samples in the Alps. The increasing worldwide contamination of soil and freshwater systems with thousands of industrial and natural chemical compounds is one of the key environmental problems facing humanity (Schwarzenbach, 2006). Although most of these compounds are present at low concentrations, many of them raise considerable toxicological concerns, particularly when present as components of complex mixtures. I frame the concerns primarily from an environmental-protection perspective with a focus on soil ecosystem in the Alps, but without neglecting the human health issues. Protecting natural waters and soils against chemical pollution safeguards soil and aquatic life and thus, directly or indirectly, human health. Hence, any measures taken to prevent the chemical pollution of surface and groundwater resources as well as soils will not only improve ecosystem health, but will also benefit both the production of clean water and safe food for human consumption

(Schwarzenbach, 2006). As an example we use a data-matrix which was generated in an international project named MONARPOP (Monitoring Network in the Alpine Region for Persistent and other Organic Pollutants) in which selected chemicals in environmental media in the mountain area of the Alps were analyzed in the years 2004 and 2005. 17 pesticides were chosen and analyzed in soil samples in Germany, Austria, Switzerland, Italy, and Slovenia. The samples were taken at 1400 m level and at other different heights (MONARPOP, 2008). The data analysis showed that chemicals like Dieldrine, Hexachlorobenzene, p,p'-DDT and p,p'-DDE showed the maximal contamination of the chosen soil samples. A further and more sophisticated method, also available in the newly developed Hasse software named PYHASSE the similarity analysis revealed that the height where the soil samples were taken has some kind of influence on the ranking of the pollutants (Voigt, 2008).

To round up the very complex topic of environmental protection, sustainable development, and risk management focussing environmental chemicals some new activities will be mentioned, like the recently founded Working Group 'Risk Management' of the Technical Committee 'Environmental Informatics' of German Society of Computer Science, GI) chaired by Alberto Susini (Working Group Risk Management, 2008). The use of non-testing methods in the risk assessment of chemicals is summed up in a special issue of the scientific journal QSAR & Combinatorial Science, edited by Andrew Worth (2008). The journal Environmental Science and Pollution Research dedicated a subject area to the topic "Risk Assessment and Management, Health" (Young, 2008).

LIST of ABBREVIATIONS

AF: Assessment Factor

DSS: Decision Support System

EDSS: Environmental Decision Support System

EUSES: European Union System for the Evaluation of Substances

GIS: Geographical Information Systems

GUI: Graphical User Interface

MONARPOP: Monitoring Network in the Alpine Region for Persistent and other Organic Pollutants

PCBs: Polychlorinated biphenyls

PEC: Predicted Environmental Concentration

PNEC: Predicted no Effect Concentration

POPs: Persistent Organic Pollutants

RCR: Risk Characterisation Ratio

REACH: Registration, Evaluation, Authorisation and Restriction of Chemicals

RMM: Risk Management Measure

SSD: Species Sensitivity Distribution

TGD: Technical Guidance Document

REFERENCES

European Commission, EUSES 2.0, the European Union System for the Evaluation of Substances. National Institute of Public Health and Environment (RIVM), Bilthoven, The Netherlands. Available through the European Chemicals Bureau, Ispra, Italy, 1998.

European Commission, Technical guidance document in support of the commission directive 93/67/EEC in risk assessment for new notified substances and the Commission regulation (EC) 1488/94 on risk assessment for existing substances. www.ecb.it, 2003.

European Commission, C Regulation (EC) No. 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/ 45/EC and repealing Council Regulation (EEC) No. 793/93 and Commission Regulation (EC) No. 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/ 105/EC and 2000/21/EC. Official Journal of the European Union, L 396/1, 2006.

Hansson, S. O., Ruden , C. Evaluating the risk decision process, *Toxicology*, 218: 100-111, 2006.

Jager, T, Vermeire, T.G., Rikken, M.G.J., van der Poel, P., Opportunities for a probabilistic risk assessment of chemicals in the European Union, *Chemosphere*, 43, 257-64, 2001.

Matthies, M., Giupponi, C., Ostendorf, B., Environmental decision support systems: Current issues, methods and tools Preface, *Environmental Modelling & Software*, 22, 123-127, 2007

MONARPOP (Monitoring Network in the Alpine Region for Persistent and other Organic Pollutants), http://www.monarpop.at/, 2008.

Richter, S. Nachhaltigkeit und Innovation im Chemikaliensektor: Welche Rollen nehmen Staat, Wissenschaft, Industrie und Verbände ein? *UWSF - Z Umweltchem Ökotox*. 20 (2), 86-89, 2008.

Schwarzenbach, Escher, B. I.; Fenner, K.; Hofstetter, T., B.; Johnson, A. C.; von Gunten, U.; Wehrli, B. The challenge of micropollutants in aquatic systems. Review. *Science*, 313: 1072-1077, 2006.

Steinhäuser KG, Greiner P, Richter S, Penning J, Angrick M., Sustainable Chemistry: Signal for Innovation or only Slogan? *ESPR – Environ Sci & Pollut Res.* 11 (5), 281-283, 2004.

United Nations. Report of the World Commission on Environment and Development, General Assembly Resolution 42/187, 11 December 1987.

United Nations General Assembly, World Summit Outcome Document, http://www.who.int/hiv/universalaccess2010/worldsummit.pdf, 15 September 2005.

Verdonck, F.A.M., Van Sprang, P.A., Vanrolleghem, P.A. An intelligent data collection tool for chemical safety/risk assessment, *Chemosphere*, 70, 1818-26, 2008.

Voigt, K., Brüggemann, R., Pudenz, S., A multi-criteria evaluation of environmental databases using the Hasse Diagram Technique (ProRank) software, *Environmental Modelling & Software*, 21 (11), 1587-1597, 2006.

Voigt K., Brüggemann, R., Schramm, K.-W., Kirchner, M., PYHASSE a New Software Tool for Partially Ordered Sets Example: Ranking of Contaminated Regions in the Alps, EnviroInfo 2008, Lüneburg, September 10. – 12., Proceedings, Shaker-Verlag, 2008, accepted.

WIKIPEDIA, Sustainability, http://en.wikipedia.org/wiki/Sustainability (06.05.08), 2008.

Working Group Risk Management, http://www.iai.fzk.de/Fachgruppe/GI/akrisk.html, 2008.

Worth, A., Computational Assessment of Toxicity and Environmental Fate, Special Issue, *QSAR & Combinatorial Science*, 27 (1), 2008.

Young, A., *Environmental Science and Pollution Research International*, Springer Verlag, 2008.