Chemicals for tomorrow

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THESIS I
The choice of products is generally dictated by ease of obtainment and technological aptitude. In the case of chemical products legal compliance and public acceptance are especially sensitive parameters for their sustainability. In order to assure legal compliance and public acceptance on the long term anyone participating in the choice of chemicals must rely on information about their inherent risks to the biosphere.

THESIS II
A transfer of knowledge from pharmaceutical and agricultural chemistry is considered to be capable of improving qualitative and quantitative understanding of Structure-Activity-Relationships SAR. The cultivation of knowledge about fate and effects of chemicals is crucial for a sustainable business process.

THESIS III
Considering the significant difficulties in conducting a scientifically sound risk assessment for a specific application emphasis has to be put on methods for low-expenditure risk analysis resulting in indicators representing persistence, spatial range, bioaccumulation, biological activity and data limitation.

LEGAL ENVIRONMENT
Sustainable Relationship

BUSINESS
Sustainable Relationship

CUSTOMER
Sustainable Relationship

BIOSPHERE

SOME THOUGHTS ON RISK INDICATORS
Persistence, defined by the global half-life of a chemical impulse, is traditionally an important argument in the evaluation of chemicals. It has to be pointed out that an estimated global half-life is far more meaningful than any half-life calculated from a degradation rate in a single environmental compound.

Spatial range as the 95%-quantile of the spatial distribution of exposures due to specific release of a chemical is a second exposure-based indicator that can be estimated by measured exposition data or by applying multi-compartment-models.

A further exposure-based indicator might be the fraction of the exposure to be found in organisms. Exact definition and development of methods for the determination of such an organismic fraction are yet to be carried through.

Due to the ongoing development of biological and ecological testing systems there is a large amount of often inhomogeneous data about effects of chemicals on organisms, organs, cells and cellular structures. Flexible aggregation of this data to an indicator for biological activity is desirable.

Data limitation is an important issue in the evaluation of ecological risks. The qualitative and quantitative limitations of available data necessary to determine the above indicators are an important measure of the uncertainty about the effects caused by the application of a chemical. Regarding ecosystem health as well as regarding human health it is true that every substance is toxic at some exposure/dose. Ignorance of the effect concentrations/doses of chemicals to be handled must be regarded as an indicator of risk.

RESEARCH AIMS
•Evaluation of performance and reliability of computer-based expert systems designed to predict fate- and effect-data
•Aggregating information from bioassays
•Case-studies for replacement chemicals
•Prediction of metabolites and analysis of their risks
•Cooperation with jurisprudence
•Considering the needs of small and medium size companies for risk analysis
•Transdisciplinary evaluation of risks

INTERDISCIPLINARY EDUCATION
•Undergraduate courses:
  „SAR of organic compounds“
  „The chemical logic of natural compounds“
•Post-graduate courses:
  „Ecotoxicology and risk assessment“

LITERATURE
Scharinger, M., 1997, Characterization of the environmental distribution behavior of organic chemicals by means of persistence and spatial range, Environmental Science & Technology, 31/10, 2891-2897