Environmental risk analysis:

Research at the University of Kalmar and the new Linnaeus University

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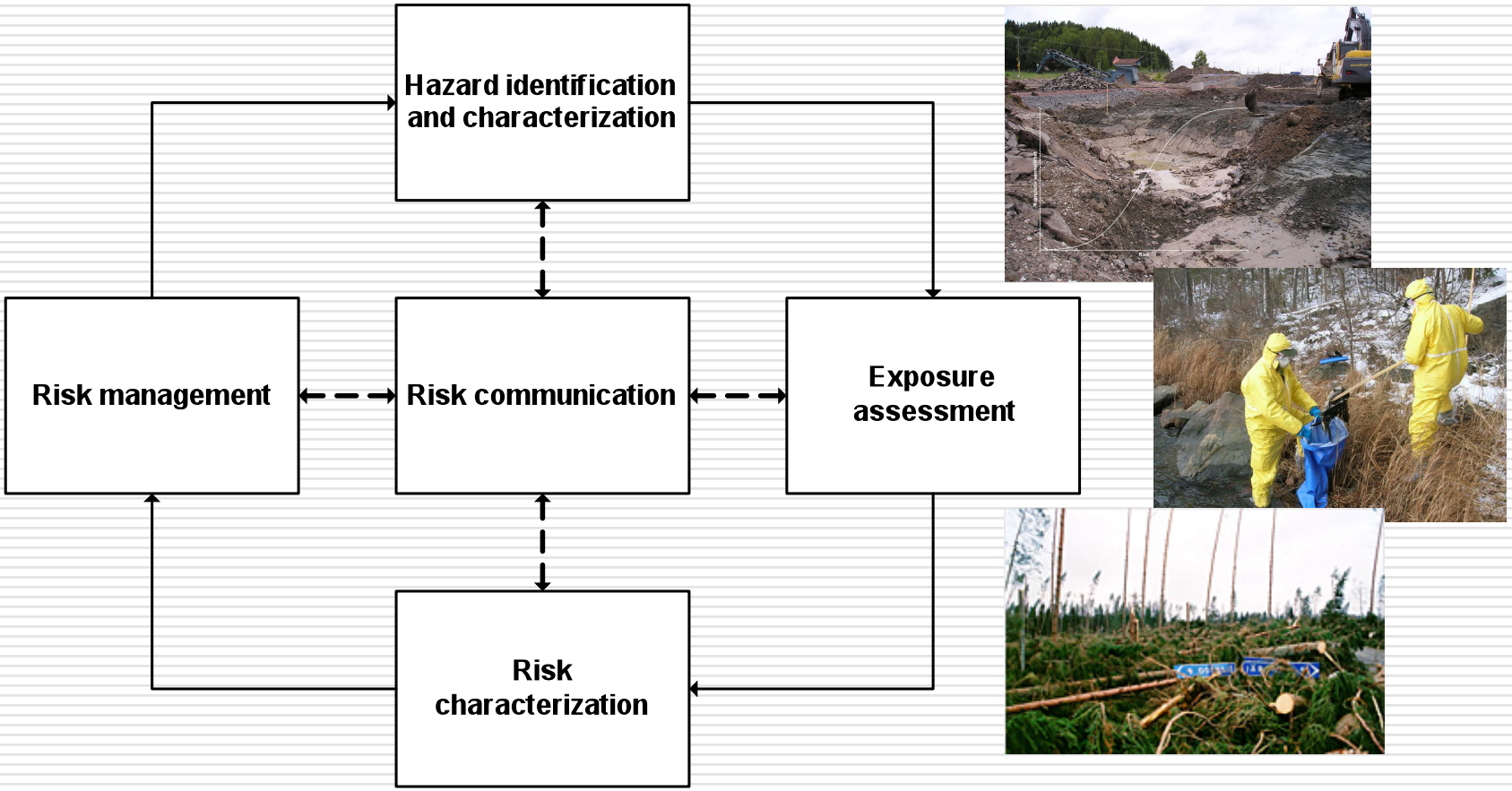
Linnæus University

Linnaeus University

- A merger of Kalmar and Växjö Universities from 2010
- 25 000 students and 2 000 employees
- School of Natural Sciences
  - 12% of staff (~200)
  - 5% of undergrad. students
  - 25% of PhD-students (~80)
  - 28% of research budget (~MSEK 100)

A risk circle to fill



Hazard identification

- Persistent organic pollutants (POPs)
  - Formation and release (emissions) from thermal processes
  - Catalytically enhanced formation and destruction
  - Distribution in the environment
- Quantitative structure-activity relationships (QSARs)
  - Biological, chemical, and physical properties
  - Virtual screening of environmentally relevant compounds
  - Method development (chemoinformatics)

Persistent organic pollutants

- Combustion, metallurgical processes, and measurement methodology
  - Process conditions and relations to process factors
  - Chemometric methods
- Catalytic formation
  - Catalytic mechanisms
  - Design of experiments
- Distribution in the environment
  - Enhanced deposition under high-voltage powerlines

QSARs: Structure-activity relationships

- Development of modelling methods
  - Domain of application
  - Local-global models
  - Model updating
- Modelling physical properties
  - Chemical and thermodynamical interpretation
- Modelling of of toxicity and degradation
  - Virtual screening of large compound libraries (data bases)
  - International cooperation

Exposure assessment and risk characterization

- Exposure factors
  - Compilation of data and meta-analysis
  - Description of variability and uncertainty in data
  - Bootstrapping
- Exposure modelling
  - Risk assessment case studies, soils and sediments
  - Mackay-type fugacity modelling (uncertainty and variability)
- Probabilistic assessment methods
  - Methods comparisons
  - Probability bounds analysis

Risk communication

- Attitudes and knowledge
  - Risk perception studies
  - Influence on communication
- Conjoint analysis
  - How preferences influence risk management decisions
  - Case studies in the steel industry
  - Methodology development (PLSR2 and L-PLS)

Some projects

- **Chemoinformatics for green chemistry** (PhD-student Tao Liu, supervisor Tomas Öberg, Faculty Board)
- **Environmental modelling and uncertainty** (PhD-student Sarfraz Iqbal, supervisor Tomas Öberg, Faculty Board)
- **The Steel Ecocycle: Attitude and knowledge – a basis for an efficient environmental communication** (PhD-student Stina Alriksson, supervisor Tomas Öberg, co-supervisor Marianne Lindström), MISTRA / Swedish Steel Producers' Association)
- **CADASTER - Case studies on the Development and Application of *in silico* Techniques for Environmental hazard and Risk assessment** (PhD-student Monika Filipsson, supervisor Tomas Öberg + postdoc to be recruited, EU 7FP)
- **ECO - Environmental ChemOinformatics**

The environmental risk analysis research group

- Senior researchers
  - Tomas Öberg, Assoc. Prof.
  - Marianne Lindström, Ph.D.
  - Post doc, to be recruited
- PhD-students
  - Stina Alriksson, M.Sc.
  - Tao Liu, M.Sc.
  - Monika Filipsson, M.Sc.
  - Sarfraz Iqbal, M.Sc.






Some recent publications

1. Öberg, T., Peltola, P. Increased deposition of polychlorinated biphenyls (PCBs) under an AC high voltage power line. *Atmospheric Environment*, in press.
2. Filipsson, M., Lindström, M., Peltola, P.. Öberg, T. Exposure to contaminated sediments during recreational activities at a public bathing place. *Journal of Hazardous Materials* 171, 200-207 (2009).
3. Liu, T., Öberg, T. Modelling of partition constants: Linear solvation energy relationships or PLS regression? *Journal of Chemometrics* 23, 254-262 (2009).
4. Tetko, I., Sushko, I., Pandey, A., Zhu, H., Tropsha, A., Papa, E., Öberg, T., Todeschini, R., Fourches, D., Varnek, A. Critical assessment of QSAR models of environmental toxicity against Tetrahymena pyriformis: Focusing on applicability domain and overfitting by variable selection. *Journal of Chemical Information and Modeling* 48, 1733-1746 (2008).
5. Cederqvist, L., Öberg, T. Reliability study of friction stir welded copper canisters containing Sweden's nuclear waste. *Reliability Engineering & System Safety* 93, 1491-1499 (2008).
6. Alriksson, S., Öberg, T. Conjoint analysis for environmental valuation - A review of methods and applications. *ESPR - Environmental Science and Pollution Research* 15, 244-257 (2008).
7. Zhu, H., Tropsha, A., Fourches, D., Varnek, A., Papa, E., Gramatica, P., Öberg, T., Dao, P., Cherkasov, A., Tetko, I. Combinational QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis. *Journal of Chemical Information and Modeling* 48, 766-784 (2008).
8. Öberg, T., Bergbäck, B., Filipsson, M. Catalytic effects by metal oxides on the formation and degradation of chlorinated aromatic compounds in fly ash. *Chemosphere* 71, 1135-1143 (2008).
9. Öberg, T., Liu, T. Global and local PLS regression models to predict vapor pressure. *QSAR & Combinatorial Science* 27, 273-279 (2008).

Teaching in environmental science

- From 2008 the basic three year BSc-program is run in parallel at campus and on the web (distance based learning)
- 1 and 2-year master programs in environmental risk analysis
  - Distance based learning (web)
  - All courses also given separately
- Environmental risk analysis is the master program in science that attracts most students

1-year masters program

- Environmental risk analysis I, 15 ECTS
- Environmental risk analysis II, 7.5 ECTS
- Environmental risk communication, 7.5 ECTS
- Degree project, 30 ECTS