ECOLOGICAL RISK ASSESSMENT (EcoRA)

Methodology, role of ICTs and its consequence for data processing

Dušek L., Holoubek I., Jarkovský J., Koptíková J., Kohout J., Šmíd R., Pavliš P., Mužík J., Hřebíček J.

Developed by RECETOX-TOCOEN & Associates, Masaryk University, Brno
Why to discuss risk assessment and environmental informatics

I. Very important and ethically binding field of application of information technologies

II. Field that relies on gathering and processing of large volume of very heterogeneous data

III. Key role of mathematics and modelling: some computational steps really determine the success of the whole methodology

IV. Key role of professional communication and information service: risk without communication is not risk

Ecological and human risk assessment is a real challenge for development of information systems, tools for automated data processing and for expert communication.
I. Role of informatics in EcoRA
II. Problem definition and conceptual model
III. Assessment scenario and endpoint selection
IV. Biological receptors and assessment endpoints
V. Parametrization of experimental data from bio-tests
VI. Monitoring of real ecosystems: model approach & strategies
ECOLOGICAL RISK ASSESSMENT

I.
Role of informatics

EcoRA methodology – process analysis – data model

Developed by RECETOX-TOCOEN & Associates, Masaryk University, Brno
Ecological risk assessment (EcoRA): key methodical steps

Problem formulation
Hazard identification

Multicomponent exposure assessment
Biological effects assessment

Risk characterization

Interpretation & Management

Validation of results

Collection & processing of data

Communication of results
EcoRA and related key information sources

Problems

Descriptive phase

Problem formulation

Libraries, databases, Information systems

Standardized tests

Modelling

Exposure assessment

Chemical monitoring

Biological effect(s) assessment

Biological monitoring

Risk characterization

Data aggregation & Synthesis

COMMUNICATION
There are many demands on information service from EcoRA.

**COMMUNICATION OF RESULTS**

- DATA
- INFORMATION
- COMMUNICATION
  - "INFLUENTIAL FACTOR"
  - "EXPOSURE"
  - "RECEPTOR"

**CHARACTERIZED RISK**

- Clear conclusions
- Value communication
- Quantified risk
- Cost analyses
- Effectiveness

Significant & verified results

Minimized uncertainties

Exact methodology

Experts

Managers

Public
Informatics: indispensable part of each methodical step

RISK CHARACTERIZATION

BIOLOGICAL EFFECTS

CONCEPTUAL MODEL & SCENARIO

EXPOSURE ASSESSMENT

Problem definition
Hazard identification

Uncertainty analysis

Sampling
Modelling
Bio-tests
Bioindicators
Biomonitoring

Model of area of interest
Experimental design

Data processing
Modelling
Multivariate analyses

Optimization
& Processing
in information systems
& Communication

Data gathering
Data aggregation
Information services

Benchmarking
Probability estimation
ECOLOGICAL RISK ASSESSMENT

II. Problem definition, conceptual model and experimental plans

Data components – database processing – conceptual model

Developed by RECETOX-TOCOEN & Associates, Masaryk University, Brno
Problem definition as obligatory entry to the assessment process

Further analyses according to scenario and formal methodology

- Are we able to prioritize key steps?
- Are we able to define sampling and measurement plan?
- Are we able to stratify the area of interest according to risk?
- Are we able to recognize risk situation?

Conceputal Model & Scenario

- Problem definition
- Hazard identification
- Retrospective problem
- Actual / urgent situation
- Prospective evaluation
Problem definition in process analysis I.

Database A.

Database B.

Database C.

National or other accepted benchmarks

Regional data sources Pilot results

Searching for information

Geographic information systems & Data processing

α_x PCB α_y

α_x PCB α_y
Problem definition in process analysis I.

Sorting – Filtering – Aggregation - Targeted searching for Information - Summary reports

PROBLEM DEFINITION & CONCEPTUAL MODEL
Ecological risk assessment SCENARIO

Exposure assessment

Biological effect(s) assessment

Risk characterization
ECOLOGICAL RISK ASSESSMENT

III. Assessment scenario and endpoint selection

Tiered analyses – situation plan – assessment scenario

Developed by RECETOX-TOCOEN & Associates, Masaryk University, Brno
Problem definition = complex information survey

Development of exact situation plan integrates also exposure assessment (at least at screening level)
Problem definition as a part of TIERED ANALYSIS

Problem definition

Source  Compounds  Situation  Area  Receptors

Pilot estimates of exposure  Situation plan

Assessment scenario

Exposure assessment  Biological effects

Chemical analyses  Information processing  Pilot biological test

TIER 1

TIER 2 ... TIER X

Chemical analyses  Biological test  Bioindicators  Ecosystem monitoring

Estimated actual (or predicted) environmental concentrations AEC  Estimated toxicological effect concentrations TEC
Problem definition generates comprehensive SITUATION PLAN ……

EXPOSURE

- Background sites with no influence of exposure
- Uncertain influence and/or uncertain assessment endpoint
- Potentially affected sites, still clean or with negligible effect
- Area with probable and substantial toxic impact
- Already strongly affected area with remarkable effects

Increasing risk

Increasing value for assessment

Priority of unit for risk assessment
and related tasks for subsequent analyses reducing uncertainty

What is the optimal and safe sampling plan?

How to minimize uncertainty in final risk estimate?

What is the optimal set of further analyses?

We need exact assessment scenario
Assessment scenario and basic principle: „Where is the problem“

Scenario is in direct relation to estimated (predicted) exposure pathways: all further analyses follow from this starting point

Primary exposure

Secondary exposure

Further tests

Stressor(s)

Time
Scenario as milestone of the assessment process

Source of contamination

Environmental characteristics

Compounds of interest

Pilot tests (screening)

Scenario

Primary exposure

Secondary exposure

SITUATION

PLAN

Further tests
IV. Biological receptors and assessment endpoints

Biological receptors – assessment endpoints – stochastic processing

Developed by RECETOX-TOCOEN & Associates, Masaryk University, Brno
Endpoint selection must follow strict rules.

Ecological relevance

Susceptibility to exposure

Reprezentativeness

Unambiguous definition

Environmental & societal importance

Accessibility for measurement

Endpoint selection must follow strict rules.
Endpoint selection: there are two basic strategies

- Stressor
  - Population
  - Communities
  - Ecosystems
  - Organisms
  - Tissue tests
  - Cell systems
  - Sub-cell systems

Bio-tests

Bio-indication
Endpoint selection: there are two basic strategies

- Model systems, biomarkers /BIO-TESTS/
- Ecosystem-related interpretation
- Both approaches must be combined in optimal way
- Biological examination provides always stochastic ("uncertain") data
- The analyses are basically multivariate

- Specificity
- Representativeness
- Monitoring of real ecosystems /BIOINDICATION/
- Mechanisms of effects
- Standardized approach
Each strategy has its advantages and disadvantages.

Interpretation

Influence of environmental factors

Time changes

Contribution to final risk estimate and its uncertainty

Suitable parameters
In final risk characterization are chemical and biological data evaluated in direct contrast.

\[ HQ = \frac{AEC}{TEC} \]

**Hazard quotient** = \( \frac{\text{Actual environmental concentration}}{\text{Toxicological effect concentration}} \)

- **Distribution 1:** Concentration of stressor in environment
- **Distribution 2:** Concentration of stressor in relation to effects
- \( X \) ? Given probability of significant negative influence (events)
- **MATC** Maximum accepted toxicant concentration (threshold)
ECOLOGICAL RISK ASSESSMENT

V. Problem 1: parametrization of experimental data from bio-tests

Dose-response curves – parameters - models

Developed by RECETOX-TOCOEN & Associates, Masaryk University, Brno
Bio-tests can be employed in any assessment step

1) Toxicological characteristics of key compounds (NOEC, LC_x data from databases)

2) Pilot (screening) tests (search for proved effects, exposure)

3) Tests in batteries
   → optimized
   → according to assessment
   → scenario (often repeated measurement)

Problem definition

Source Compounds Situation Area Receptors

Pilot estimates of exposure

Situation plan

Assessment scenario

Exposure assessment Biological effects

Chemical sampling Ecosystem monitoring In situ bioindicators Analyses of biota Biological tests Exposure models

Estimated actual (or predicted) environmental concentrations AEC

Estimated toxicological effect concentrations TEC

TIER 1

TIER 2 .... TIER X
Standard output of bio-tests: dose-response curve

- „Low-effect“ concentrations

**NOEC**: No Observed Effect Concentration

-> the highest concentration of a chemical in a toxicity test that causes effects that are not statistically significant from control

**LOEC**: Lowest Observed Effect Concentration

-> the lowest concentration of a chemical in a toxicity test that causes effects that are statistically significant from control

- „X – effect“ concentrations

**LD$_{50}$, LC$_{50}$, LD$_X$, LC$_X$**

-> Median lethal dose (concentration), X-effect lethal dose (concentration)
Dose-response problem in its textbook form

Standard experimental design → Standard dose-response curve

- Control
- Concentration X1
- Concentration X2
- Concentration X3
- Concentration Xp

Growing concentration of tested compounds

- Applied concentration levels of tested compound
- Model estimates and extrapolation between doses
- NOEC, LOEC
- L(E,I)C_{50}
- LC_{x}, EC_{x}, IC_{x}

Straightforward comparison of experimental variants
Dose-response problem in its textbook form

Comparative approach

Model approach

Asking the Right Questions:
Ecotoxicology and Statistics.

Statistical Analysis of Aquatic
Toxicity Data. OECD Workshop.
Braunschweig, 1996

NOEC / LOEC approach criticized and refused: low standard of estimates, dependent on experimental design, low extrapolation potential

Preferred way: dose-response models and extracted LC$_X$ (EC$_X$)

Model solution for dose-response modelling: regression

Model regression standards: example

**Estimate of EC**

\[ Y = \frac{\alpha}{1 + \left(\frac{p}{1-p}\right)e^{\beta(x - \mu_p)}} \]

\( x = \ln \text{(koncentrace)} \)
\( \mu_p = \ln \text{ED}_p \)

**Estimate of threshold concentration**

\[ Y = \frac{\alpha}{1 + \left(\frac{p}{1-p}\right)e^{\beta[(x - \mu_o) - (\mu_p - \mu_o)]}} \]

\( x = \ln \text{(koncentrace)} \)
\( \mu_p = \ln \text{ED}_p \)
\( \mu_o = \ln \text{ED}_o \)

**Evaluation of hormesis model**

\[ Y = \frac{\alpha + \delta x}{1 + \left(\frac{p}{1-p}\right)e^{\beta(\ln x - g)}} \]

\( x = \text{koncentrace} \)
\( \mu_o = \ln \text{ED}_o \)

**OECD, 1996 - 1999**

\[ Y = B \left( \sqrt{C^2 - \left(\frac{X - X_0}{A}\right)^2} + Y_0 \right) \]

+ resistance estimate
„Real“ dose response problem: bio-tests in environmental matrices

Patterns of various dose response data: examples

REZISTENCE
LAG & HORMESIS
SIGMOIDITY
SUSCEPTIBILITY
“Real“ dose response problem: bio-tests in environmental matrices


We need robust model tools to estimate the patterns and associated parameters.
Median effect equation: theoretical background

\[ \frac{F_A}{F_N} = \left( \frac{C}{EC_{50}} \right)^m \]

\[ \log \left( \frac{F_A}{F_N} \right) = m \log(C) - m \log(EC_{50}) \]

\[ \text{Pro } F_A = F_N = 0.5: \]
\[ \frac{[m \log(C_i)]}{m} = \log(EC_{50}) \]

\[ F_A = \frac{1}{[1 + (EC_{50}/C)]^m} \]

\[ C = EC_{50} \left[ F_A / (1 - F_A) \right]^{1/m} \]

\( F_A, F_N \) – fraction of affected subjects, individuals, cells, ....

\( C \) – concentration of applied compounds

\( M \) – estimated coefficient (related to sigmoidity of the curve)

\( EC_{50} \) – median effect concentration

Chou. T.C. 1980 - 1989

Carcinogenesis;
Trends in Pharm. Res.
V. Problem 2: monitoring of real ecosystems: model approach and strategies

Biondication – reference sites – analog modelling
Biondication and ecosystem monitoring in tiered analysis

**Problem definition**

- **Source**
- **Compounds**
- **Situation**
- **Area**
- **Receptors**

**Pilot estimates of exposure**

**Situation plan**

**Assessment scenario**

**Exposure assessment**

- Chemical sampling
- Ecosystem monitoring
- In situ bioindicators
- Analyses of biota
- Biological tests
- Exposure models

**Biological effects**

**Key environmental data from the area of interest**

1) Evidence of toxic impacts in past

2) Benchmarking for the status of valuable ecosystems

**Estimated actual (or predicted) environmental concentrations AEC**

**Estimated toxicological effect concentrations TEC**
Biomonitoring of ecosystems: very complex multivariate data

Rather than confidence estimates from repeated trials we apply searching for analog situation (sites)

Analog modelling for ecological risk assessment

A) Calibration data set

Contaminated sites

\[ X_1, X_2, X_3, \ldots, X_p \]

Reference (clean) sites

\[ X_1, X_2, X_3, \ldots, X_p \]

New problem

Searching for similarities

B) Environmental gradient

Increasing disturbance

Increasing contamination

Gradient calibration

New problem

Searching for similarities

RISK ASSESSMENT SCENARIO
Clustering of sites /aggregation criteria/

Searching for relevant reference sites

Definition of representative sites for detailed studies

„Natural / evolutionary" background of the sites in contrast to ecotoxicological and/or chemical measures: is there any added value?
Analog modelling for ecological risk assessment: strategy

(1) Representative biomonitoring network

(2) Other available data

(3) „Centroids of groups“

- Representative information background
  - abiotic determinants
  - biotic descriptors

- Basic typology of sites
  - Ecologically-related clustering

- Selected set of sites, suitable and interesting for mutual comparisons (candidates for reference sites, representative minimized network, ..........)

- Additional characteristics leading to agreement or disagreement with general characteristics

- Ecotoxicological and chemical measures
Analog modelling for ecological risk assessment: strategy

Typology of sites

Representatives of different types of sites

Searching for reference sites

Verification/definition of reference points

Investigative typology of sites

Set of similar sites (variability study)

DESIGN + SCENARIO of EcoRA