Mechanistic Effect Models for Ecological Risk Assessment of Chemicals: CREAM and the Documentation Framework TRACE

Volker Grimm

HELMHOLTZ
ZENTRUM FÜR
UMWELTFORSCHUNG
UFZ

CONTENTS

HELMHOLTZ
ZENTRUM FÜR
UMWELTFORSCHUNG
UFZ

The protection goal in most directives are sustainable populations:

"does not have any long-term repercussions for the abundance and diversity of non-target species" (EU Dir 91/414).

Population-level effects of chemicals depend on:

- **Exposure and toxicity**
- **Ecological factors:**

  Life history characteristics, population structure, density dependence, exposure patterns, landscape structure, interactions

ECOLOGICAL RISK ASSESSMENT (ERA)

„Ecological risk assessment is a science-based process that can be used to evaluate the likelihood that **adverse ecological effects** can result from exposure to stressors in the environment.“

Munns (2006)

HELMHOLTZ
ZENTRUM FÜR
UMWELTFORSCHUNG
UFZ

CURRENT RISK ASSESSMENT (RA)

- Focussed on **individual** in the lab
- **Hard to extrapolate** to population level
- What are **effects** on populations?
- Will populations **recover**?
- Current RA includes **little ecology**

EMPIRICAL APPROACHES: LIMITATIONS

Mesocosm experiments and field studies

- **Extrapolation** to other species?
- **Extrapolation** to other environments?
- Number of replicates: **significant** effects?
- **Understanding**: controlled experiments
- Usually, **scales** too large and **complexity** often too high
- **Interactions?**

HELMHOLTZ
ZENTRUM FÜR
UMWELTFORSCHUNG
UFZ

POPULATION MODELS

- Purposeful, simplified **representations** of real populations
- Try to capture **essential** structures and mechanisms
- Often are implemented as **computer simulations**
- Once they are sufficiently **validated**, they can be used to overcome limitations of standard tests and experiments

POTENTIAL OF POPULATION MODELS

- **Virtual laboratory**
- **Understanding**: controlled experiments
- **Extrapolation** from individual to population
- **Extrapolation** to other species?
- **Extrapolation** to other environments
- **Interactions**


CD-ROM INCLUDED
Demographic Toxicity
Methods in Ecological Risk Ass
Population-Level Ecological Risk Assessment
Lawrence W. Barn
Wayne R. Munns,
Mary T. Sorensen
EPA/100/R-09/006 | October 2009
www.epa.gov/osa
EPA
United States Environmental Protection Agency
Summary Report:
Risk Assessment Forum Technical Workshop on Population-level Ecological Risk Assessment
WILDLIFE TOXICOLOGY and POPULATION MODELING
Integrated Studies of Agroecosystems
Edited by
Ronald J. Kendall and
Thomas E. Lacher, Jr.
A Special Publication of SETAC
Ecological Modeling in Risk Assessment
Chemical Effects on Populati
Ecosystems, and Landscapes
Edited by
Robert A. Pastorok
Steven M. Bartell
Scott Ferson
Lev R. Ginzburg
LEWIS PUBLISHERS
Ecological Models for Regulatory Risk Assessments of Pesticides
Developing a Strategy for the Future
Edited by
Pernille Thorbek, Valery E. Forbes, Fred Heimbach,
Udo Hommen, Hans-Hermann Thulke, Paul J. Van den Brink,
Jörn Wogram, Volker Grimm

CURRENT MODELLING PRACTICE

Environmental Toxicology and Chemistry, Vol. 29, No. 4, pp. 1006–1012, 2010
© 2010 SETAC
Printed in the USA
DOI: 10.1002/etc.120

Hazard/Risk Assessment

ECOLOGICAL MODELS AND PESTICIDE RISK ASSESSMENT:
CURRENT MODELING PRACTICE

AMELIE SCHMOLKE,*† PERNILLE THORBEK,‡ PETER CHAPMAN,‡ and VOLKER GRIMM†
†UFZ, Helmholtz Centre for Environmental Research, Department of Ecological Modelling, Permoserstraße 15, 04318 Leipzig, Germany
‡Syngenta, Environmental Safety, Jealott's Hill International Research Centre, Bracknell, Berkshire RG42 6EY, United Kingdom

(*Submitted* 14 *May* 2009; *Returned for Revision* 27 *July* 2009; *Accepted* 3 *November* 2009)

Abstract—Ecological risk assessments of pesticides usually focus on risk at the level of individuals, and are carried out by comparing exposure and toxicological endpoints. However, in most cases the protection goal is populations rather than individuals. On the population level, effects of pesticides depend not only on exposure and toxicity, but also on factors such as life history characteristics, population structure, timing of application, presence of refuges in time and space, and landscape structure. Ecological models can integrate such factors and have the potential to become important tools for the prediction of population-level effects of exposure to

- **Many scientific papers**
- **Most of them unsuitable for regulatory risk assessment**

CURRENT MODELLING PRACTICE

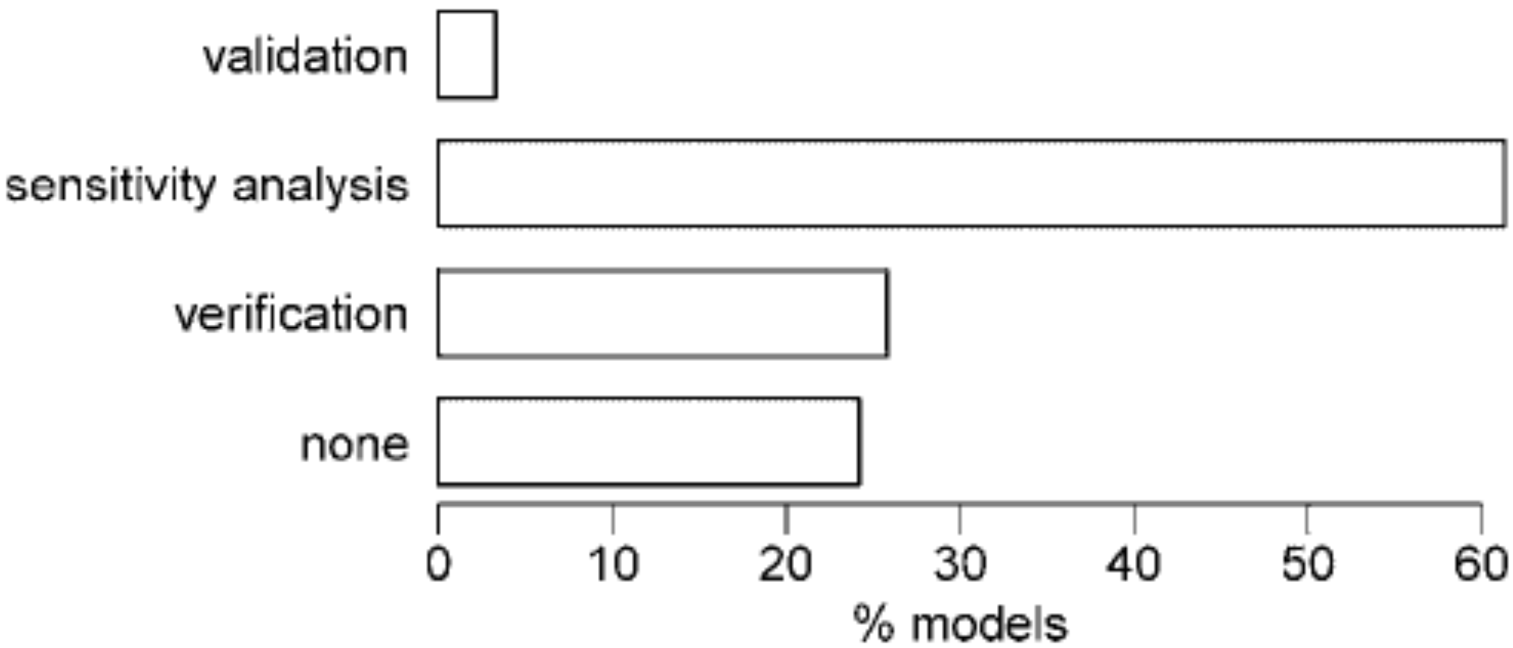


Fig. 6. Model evaluation. Some models were subject to multiple evaluation methods.

- **Little testing: so why should trust these models?**

CURRENT MODELLING PRACTICE

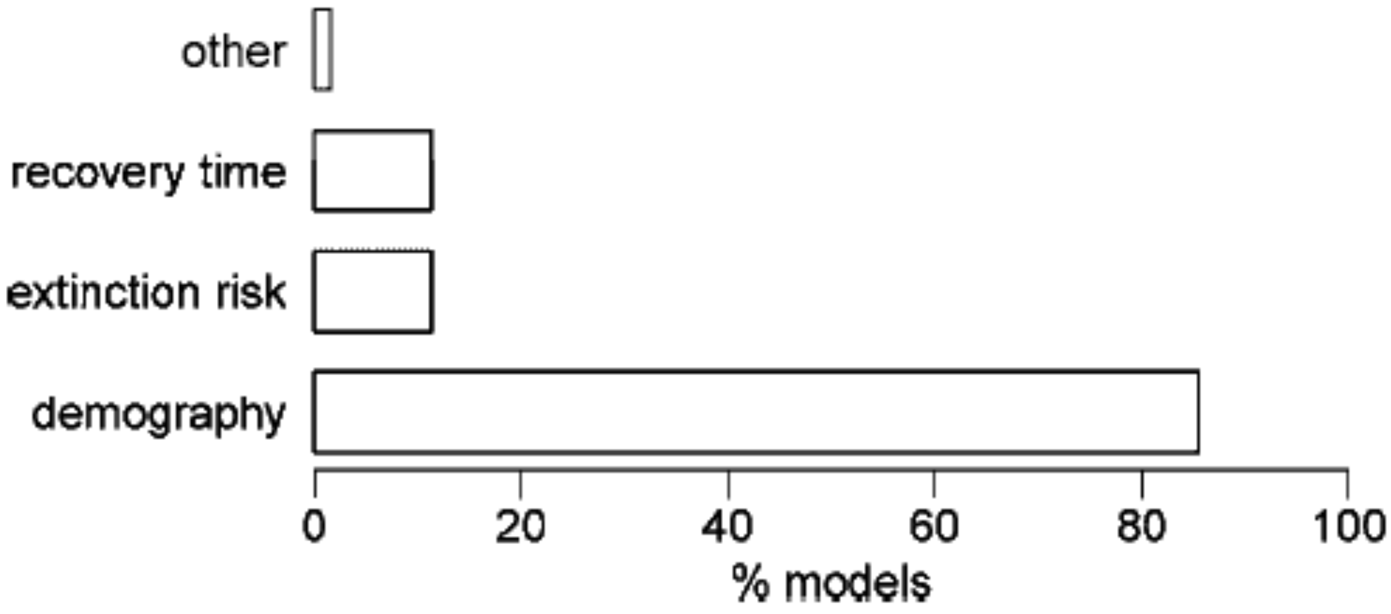
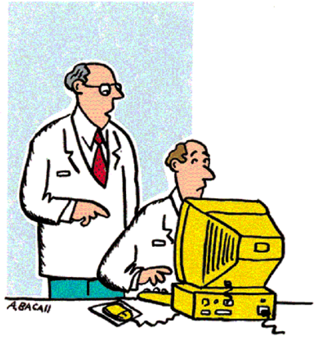


Fig. 4. Endpoint of risk assessment. Most models provided demographic results, mostly population growth rate or size. Models may include more than one endpoint.

- **Most endpoints considered are unsuitable for risk assessment**

CHALLENGES



Modellers (academia):

- How can I **publish** my model?
- Would there be regulators who know modelling?
- **What do regulators need, want, or expect**?

Industry:

- Should we **invest** in modelling and modellers?
- Do we need to be **prepared** for increasing demand for ERA?
- Will effect models and ERA make things **easier** or more **complicated**?

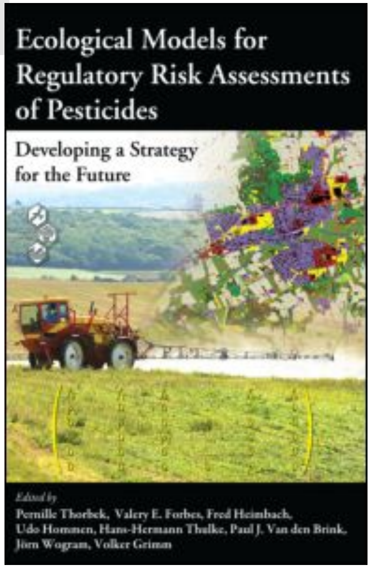
Regulators:

- How can we understand the model?
- **What** is the model?
- How **uncertain** is it?
- Why so many different model types?
- How could we assess the suitability of models for ecological risk assessment?
- Can models lead to **better RA**?
- **Why should we trust models**?

TWO OBSTACLES TO WIDER USE OF MODELS

- The lack of a framework for developing mechanistic effect models in a regulatory context in a coherent and transparent way
- The lack of researchers that are well-trained both in ecological modelling and risk assessment.

LEMTOX



Mechanistic Effect Models for Ecological Risk Assessment of Chemicals

Marie Curie Initial Training Network (ITN)

European Commision (7th FP)

September 2009 – August 2013

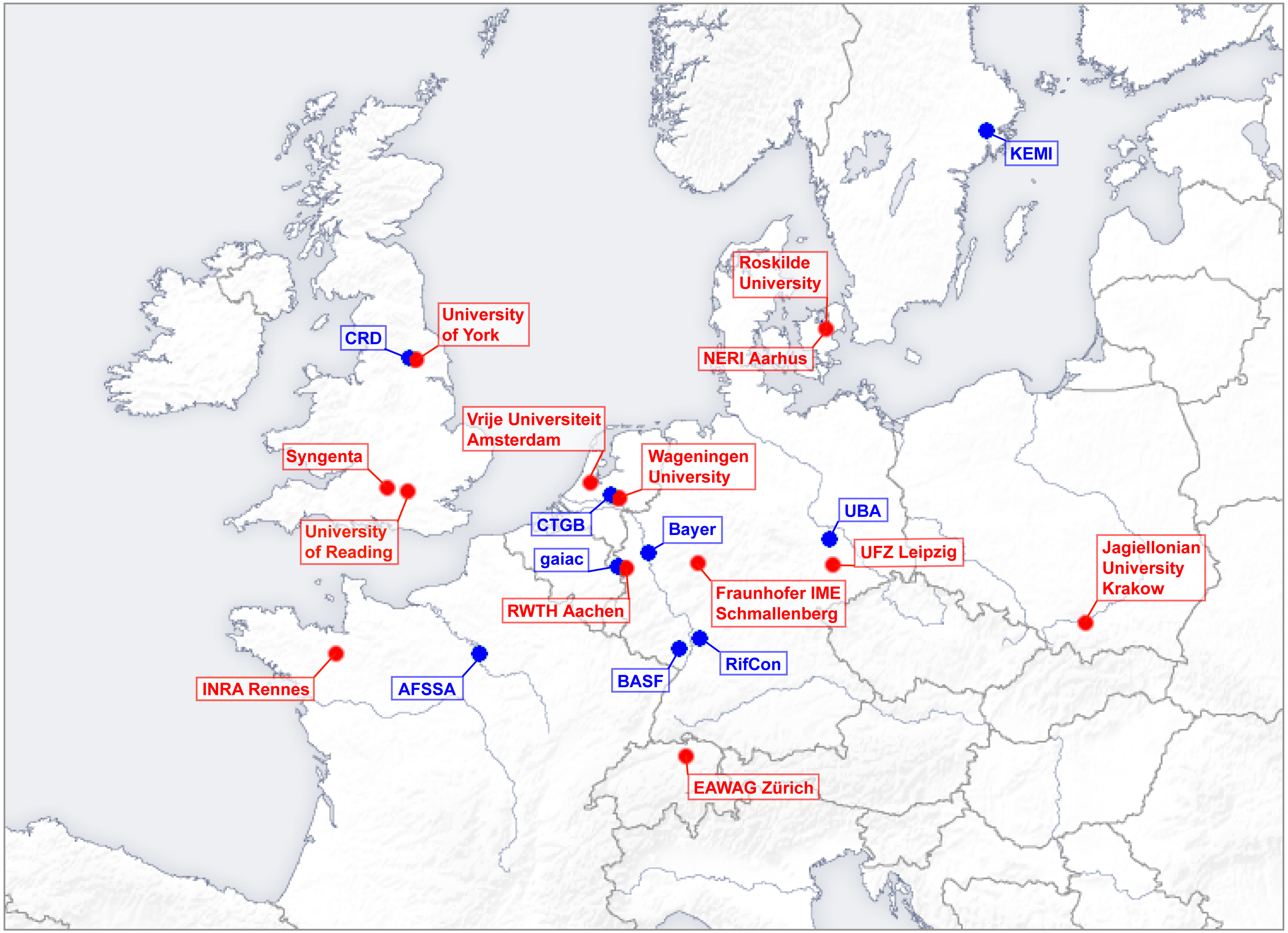
http://cream-itn.eu

AIMS AND SCOPE OF CREAM

1. **Train** young researchers in modelling and chemical risk assessment
2. Develop and test **models for chemical risk assessment**
3. Develop **guidance for good modeling practice** in chemical risk assessment with regulators, industry, and academia

HELMHOLTZ
ZENTRUM FÜR
UMWELTFORSCHUNG
UFZ

TRAINING NETWORK



23 FELLOWS – 13 PARTNERS – 9 ASSOCIATED PARTNERS

GOOD MODELLING PRACTICE: REVIEW

We evaluated **41 publications:**

- Species management/conservation biology (11)
- Fisheries and marine ecosystem managment (4)
- Forest and land use management (5)
- Natural resource management (9)
- Pest management (2)
- Chemical risk assessment (5)

Review

Cell PRESS

Ecological models supporting environmental decision making: a strategy for the future

Amelie Schmolke[1], Pernille Thorbek[2], Donald L. DeAngelis[3] and Volker Grimm[1]

[1] UFZ, Helmholtz Centre for Environmental Research – UFZ, Department of Ecological Modelling, Permoserstr. 15, 04318 Leipzig, Germany
[2] Syngenta, Environmental Safety, Jealott's Hill International Research Centre, Bracknell, Berkshire RG42 6EY, UK
[3] USGS/Biological Resources Division and Department of Biology, University of Miami, PO Box 249118, Coral Gables, FL 33124, USA

Ecological models are important for environmental decision support because they allow the consequences of alternative policies and management scenarios to be explored. However, current modeling practice is unsatisfactory. A literature review shows that the elements of good modeling practice have long been identified but

Although ecological models have been used to support some environmental decision making for a long time, we think that they will need to be used much more widely in the future. This trend is confirmed by the increasing interest shown by authorities and industry in ecological models and their applications [9–11]. In addition, it is

Schmolke A, Thorbek P, DeAngelis DL, Grimm V. 2010. *Trends in Ecology and Evolution* 25: 479-486

CONVERGENT ISSUES

Elements of the modeling process that were considered critical for the role of ecological models for supporting environmental decision making

- **13 convergent issues**

Table 1. Elements of good modeling practice identified from the literature

Element	Description	References[a]
Inclusion of stakeholders	Ongoing communication between stakeholders and modelers during model building, which is a critical factor for the success or failure of modeling projects.	[19,27,31,32,38–40,49,50]
Formulation of objectives	Definition of objectives at the outset of a modeling project, which includes the assessment of the actual management issue, key variables and processes, data availability, kind of outputs required, and how they will inform decisions.	[17,19,28–32,38,39,49,51–54]
Conceptual model	Formalization of the assumptions about the system and preliminary understanding of its internal organization and operation.	[19,21,31,32,39,49,54]
Choice of model approach	Identification of the most appropriate modeling approach in the context of the goal of the modeling project.	[18–21,31,49,51,52,55–58]
Choice of model complexity	Determination of the optimal complexity level for the problem at hand.	[19,27,31,51,53,55,56,58–62]
Use of multiple models	Application of multiple models to the same problem, which can decrease the uncertainty about the appropriate model approach and main assumptions.	[17,31,41,55,58,63]
Parameterization and calibration	Determination of model parameters from empirical data or by means of calibration of the model outputs on the basis of data.	[17–21,30–32,41,49,55,57,58,60,64,65]
Verification	Assurance that the modeling formalism is correct; i.e., that the model has been implemented correctly.	[17,19–21,28,31,66,67]
Sensitivity analysis	Systematic testing of the sensitivity of model results to changes in parameter values.	[17,20,28–32,39,41,53,55,68,69]
Quantification of uncertainties	Determination of the confidence limits of the model outputs, which is essential for the judgment of the usefulness of the model and its outputs in the contexts of decisions.	[19,21,22,30–32,41,53,54,58,65,68–72]
Validation	Comparison of model outputs with independent empirical data sets; i.e., data that have not been used for parameterization or calibration of the model.	[17,19–22,28–31,54,55,58,65,67,68,70]
Peer review	Quality assessment of a model and its analyses by independent experts.	[17,28,31,39]
Documentation and transparency	Accurate communication of models, and transparency of the modeling process, which can be achieved through a clear and complete documentation of the model and its evaluation.	[6,7,20,27–31,39,50,65,68,72]

LESSONS FROM REVIEW

- Elements of Good Modelling Practice **are all there** and well-known, in principle
- Very good attempts to provide guidance already exist (EPA; also in hydrological modelling)

THE REAL PROBLEM IS

- **NOT** so much defining (guidance for) Good Modelling Practice
- **BUT** getting this practice – into practice

WHY IS THIS SO?

- Lack of inclusion of stakeholders
- Lack of incentives for modellers to follow good practice
- Inconsistent terminology

BASIC IDEA

Instead of:

Do the right thing!

Document the right thing!

Establish a standard for documenting models, their development, and their analysis

We are familiar with such standards

Title

Abstract

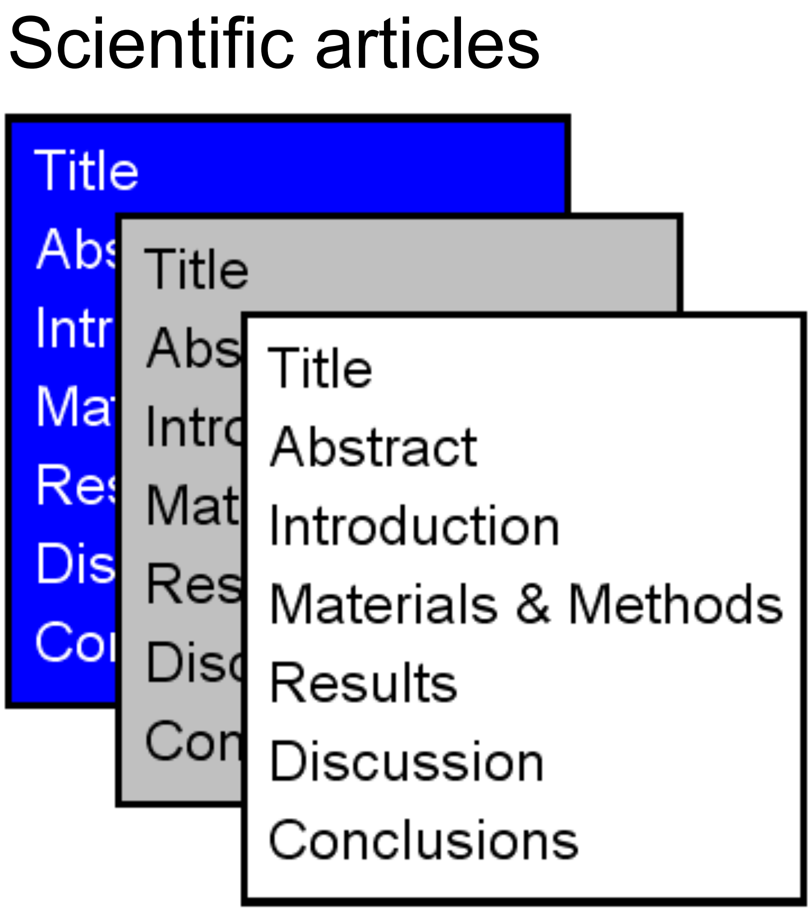
Introduction

Materials and Methods

Results

Discussion

Conclusions



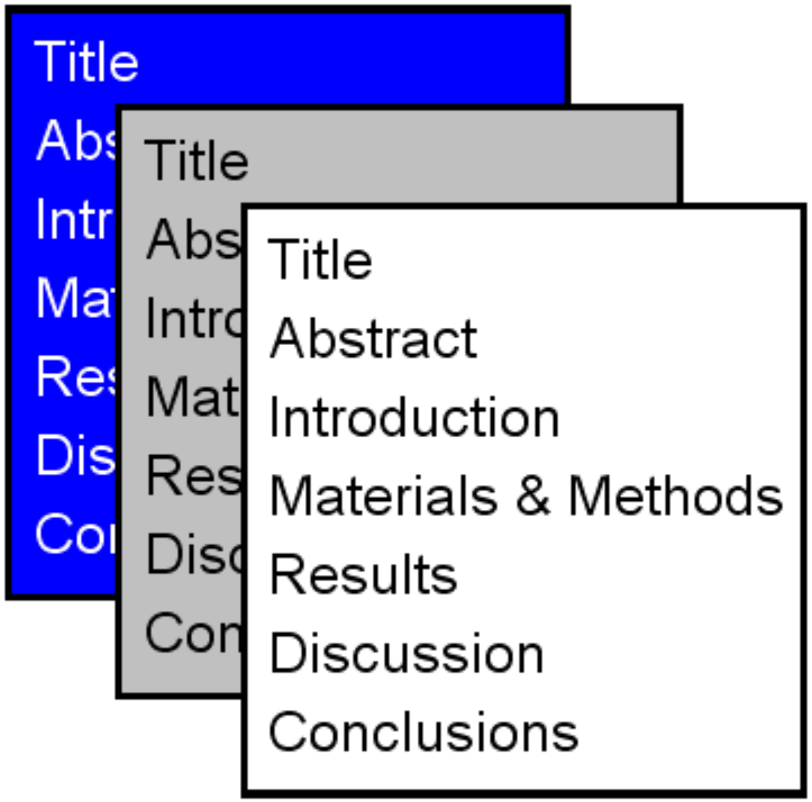
Benefits of standards

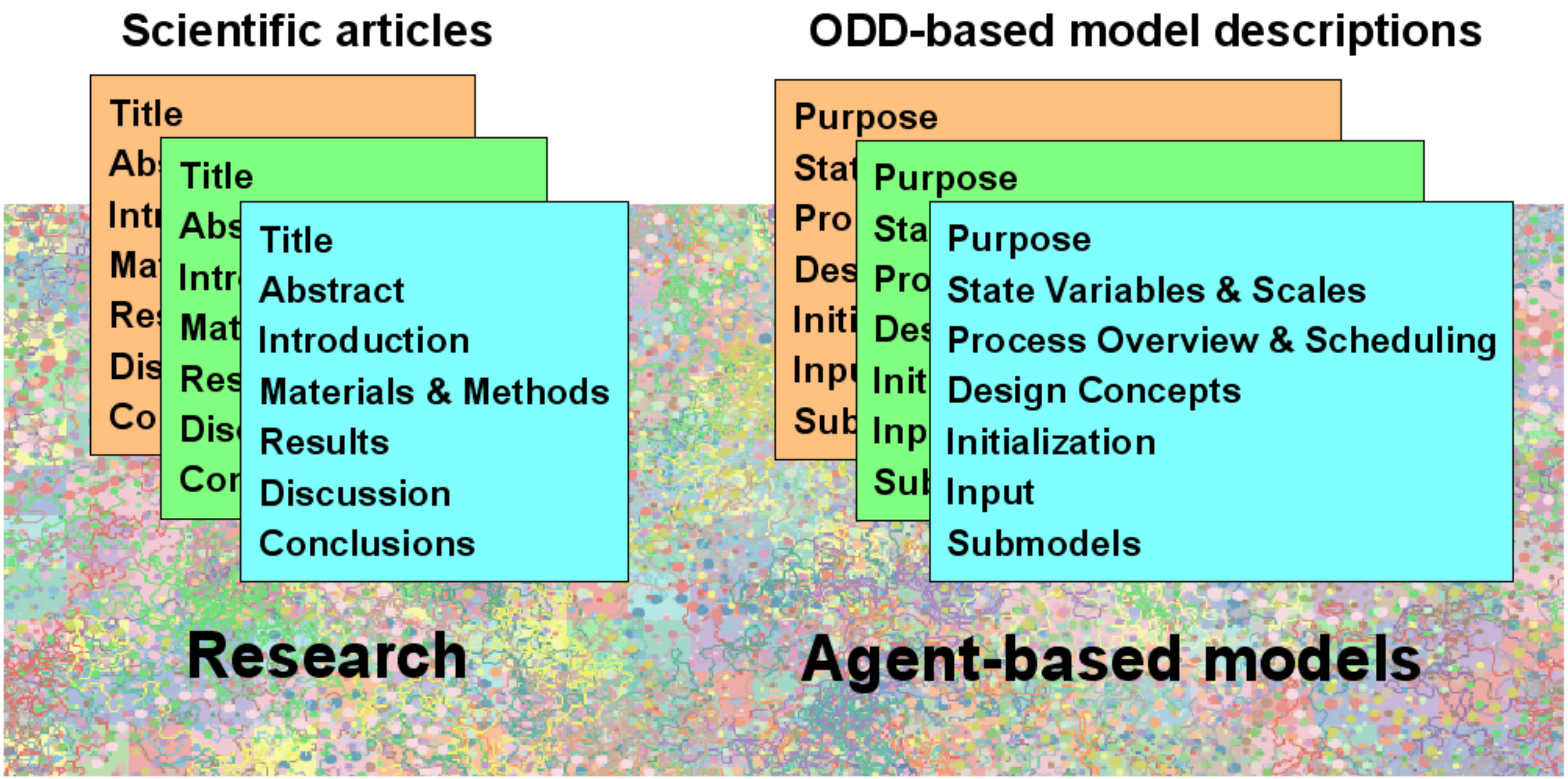
- **Increase efficiency and coherence**
- **Do things in a more systematic way**
- **Provide checklists**
- **Facilitate communication**
- **Facilitate design**

Standards <u>must not</u>:

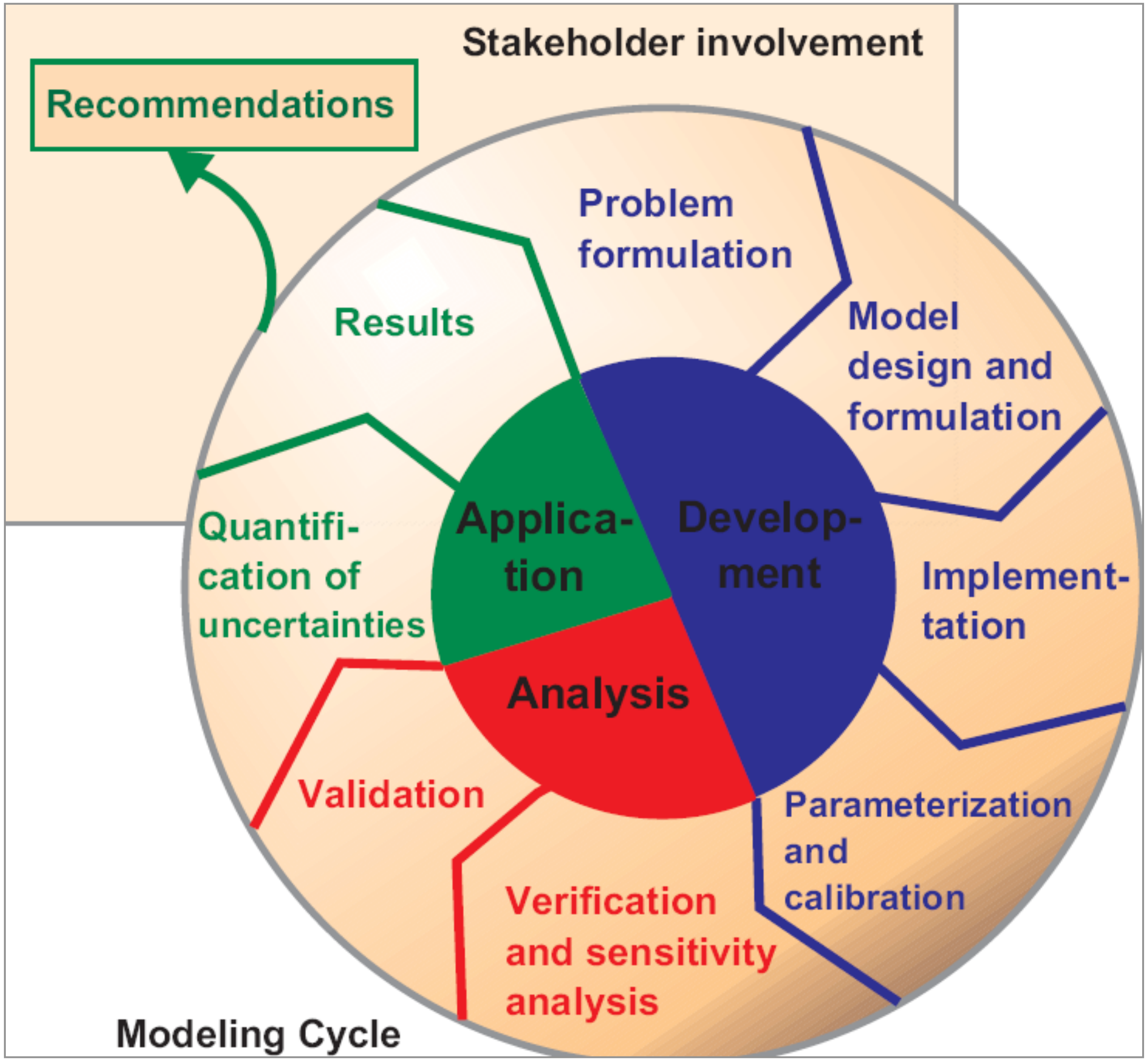
- **Impose designs**
- **Limit creativity**

Scientific articles




Scientific articles
ODD-based model descriptions
Title
Abstract
Introduction
Materials & Methods
Results
Discussion
Conclusions
Purpose
State Variables & Scales
Process Overview & Scheduling
Design Concepts
Initialization
Input
Submodels
Research
Agent-based models

BASIS OF STANDARD: THE MODELING CYCLE



Box 1. TRACE (transparent and comprehensive ecological modeling) documentation structure

I. Model development

Problem formulation: *Context* in which the model will be used, and the type of audience addressed; *specification of the question(s)* that should be answered with the model; statement of the *domain of applicability* of the model, including the extent of acceptable extrapolations; assessment of the *availability of knowledge and data*; specification of necessary *model outputs.*

Design and formulation: Description of the *conceptual model*; description and justification of the *modeling approach* used and of the *complexity*; *entities and processes represented* in the model; most important, the applied *assumptions* about the system.

Model description: Detailed *description of the actual model* and how it has been *implemented* (programs, software platforms, scripts).

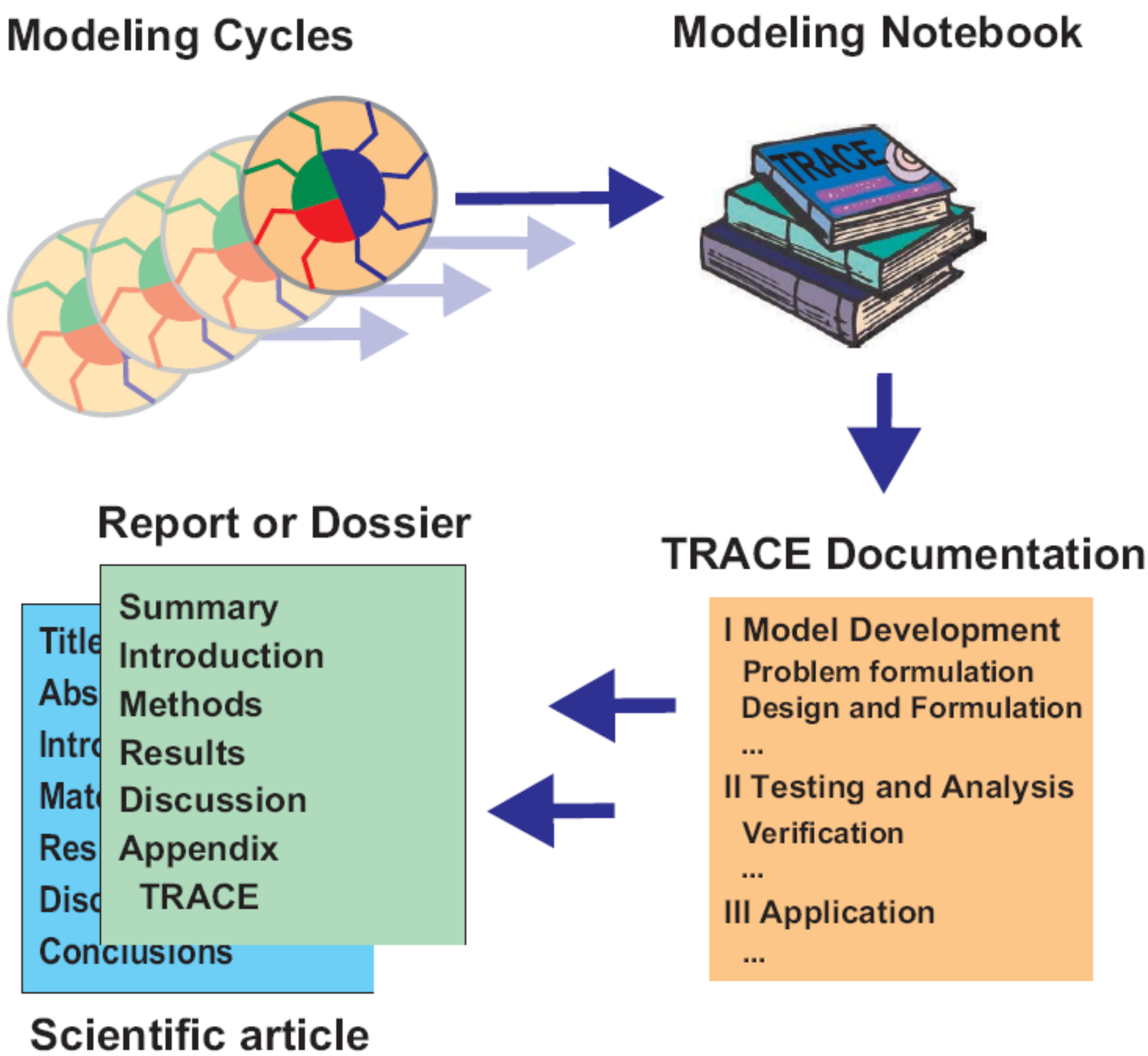
Parameterization: *List of all parameter values* used in the model, the *data sources*, and how the parameter values were obtained or calculated; *uncertainties* associated with each parameter.

Calibration: Documentation of the *data sets used* for calibration; *which parameters* were calibrated; what *optimization method* was used.

II. Model testing and analysis

Verification: Assessment of whether the model is working according to its specifications; documentation of what tests have been conducted.

Sensitivity analysis: Exploration of the model behavior for *varying parameters*; documentation of which *parameter combinations* have



Modeling Cycles
Modeling Notebook
TRACE
Report or Dossier
TRACE Documentation
Title
Abs
Intro
Mat
Res
Disc
Conclusions
Summary
Introduction
Methods
Results
Discussion
Appendix
TRACE
I Model Development
Problem formulation
Design and Formulation
...
II Testing and Analysis
Verification
...
III Application
...
Scientific article

EXAMPLE MODEL: COMMON SHREW

Developed by **Magnus Wang** (**RifCon**, Germany)

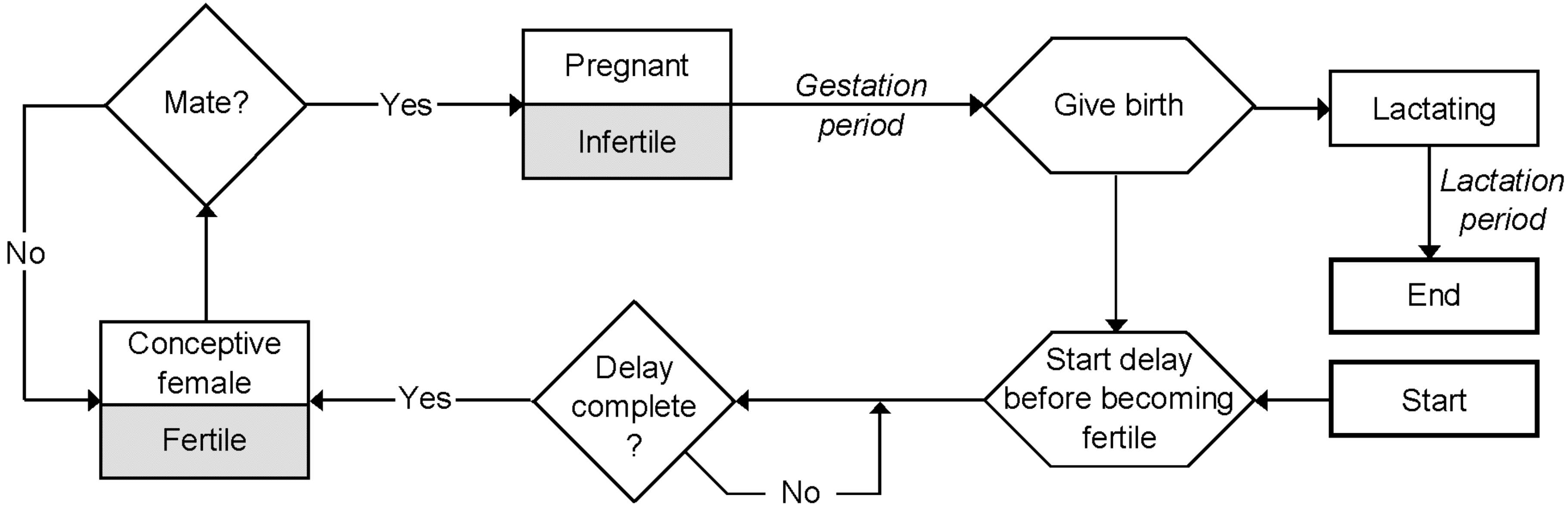
- **Landscape**: grid cells (5m), 100x100
- **Grid cells**: habitat type and quality (resources)
- **Individuals**: age, sex, stage, reproductive status, ID of home range
- **Home range**: list of grid cells, ID of owner

Wang & Grimm (2007) Ecological Modelling 205: 397-409
Wang & Grimm (2010) Environmental Toxicology and Chemistry 29: 1292-1300.

RIFCON GMBH

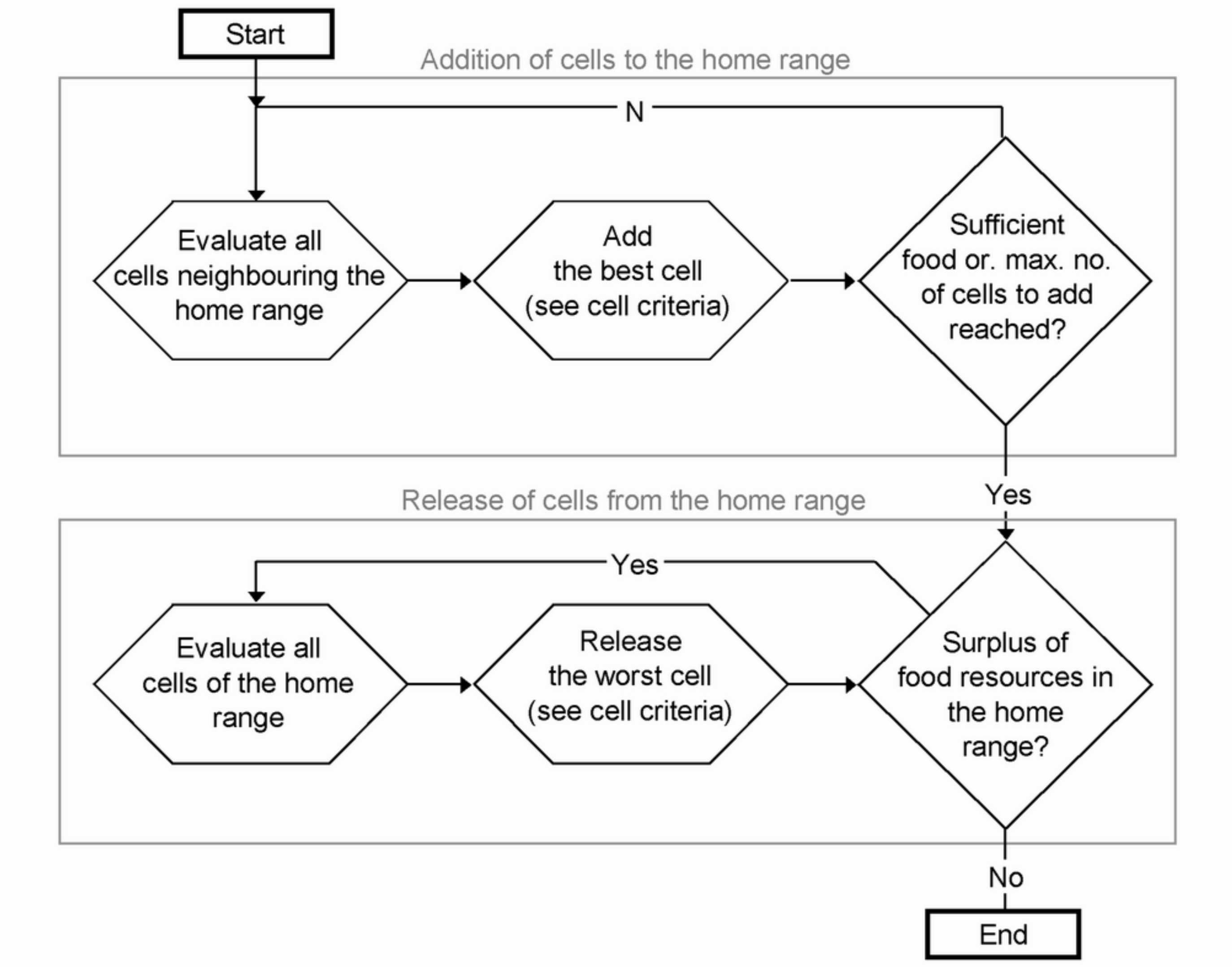
Individual-based model

Follow life cycle and behaviour of each individual



Key behaviour

Territoriality → spatially explicit model



Example: Patterns for testing and validation

Size, distribution, and dynamics of territories

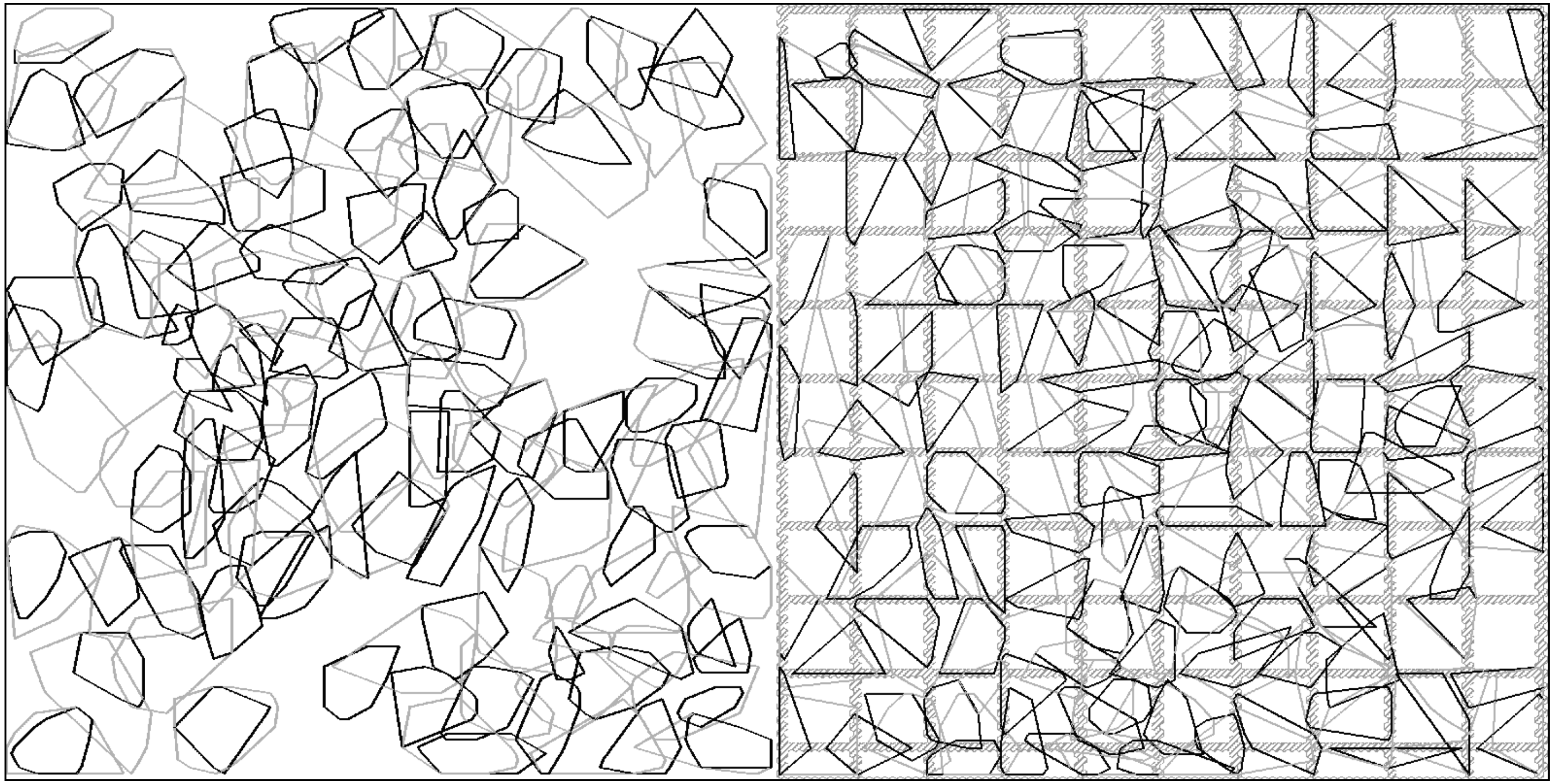
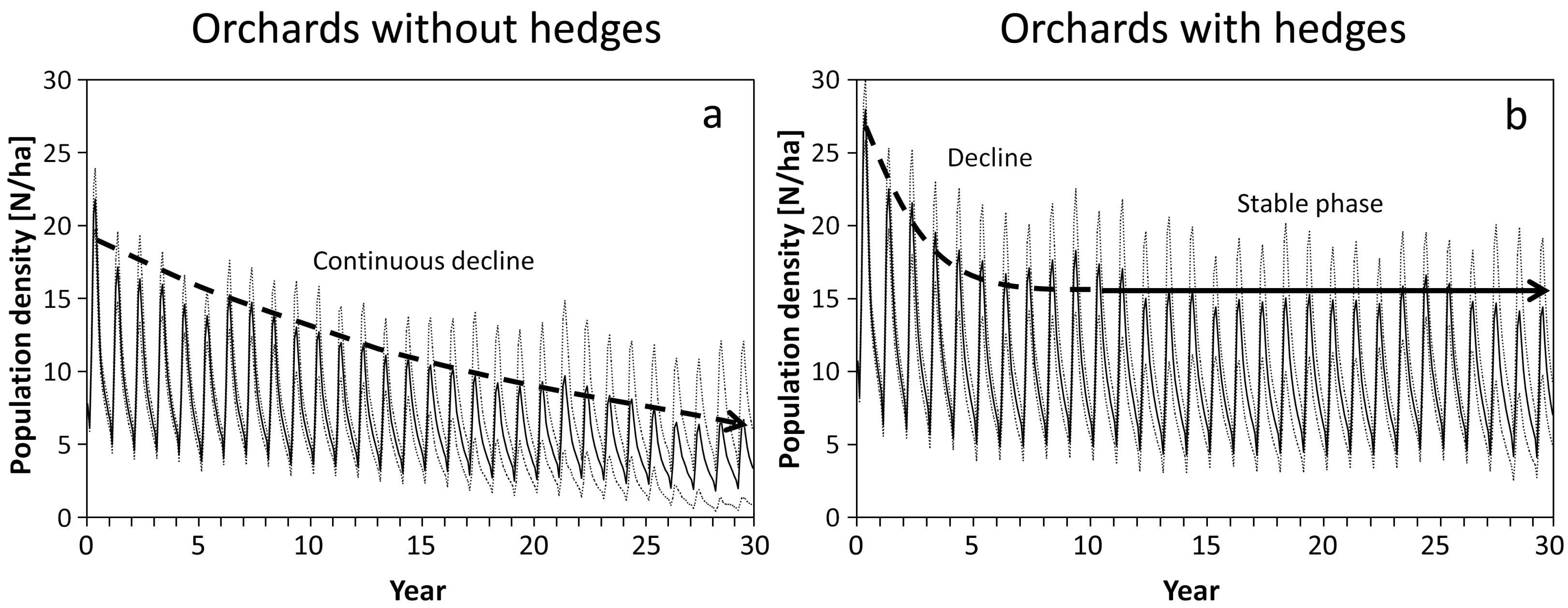


Table 4 – Key-variables for model testing

Examples of variables for model validation	Model output	Values from literature	Reference
Reproduction			
Number of litters per female lifetime	2	1–2	Churchfield (1990)
Percentage of pregnant or lactating females	82.6–100%	Up to 90% or more	Churchfield (1990)
Age distributions (percent juveniles/subadults at the begin of the population increase)	First month: 39.7% Second month: 74.4% Third month: 85.3%	First month: 35.8% Second month: 63.2% Third month: 84.4%	Calculated from Churchfield et al. (1995)
Survival			
Survival rates	Month Rate/month 1–2 0.784 3–13 0.914 ≥14 0.544	Month Rate/month 1–2 0.645 3–13 0.850 ≥14 0.333	Churchfield et al. (1995)
Life spans	Maximum 15 months	Maximum 15 months	Churchfield (1990)
Age distributions	See above	See above	See above
Spatial distribution			
Home range sizes	Subadult: 490 m^2 Females: 1027 m^2 Males: 2361 m^2	Subadult: 526 m^2 Males: – Females: –	Michielsen (1966) No references for adult *S. araneus*, but 2× and 4× increase reported for female and male *S. vagrans* (Hawes, 1977)
Percentage of dispersers	Up to 35	–	–
Population dynamics			
Timing of population peak	June–August	May–September	Michielsen (1966), Churchfield (1980) and Churchfield et al. (1997)
Fluctuations of maximum density	−72.1 to +109.6%	−38.6 to +118.5%	Michielsen (1966), Pernetta (1977), Churchfield (1980) and Churchfield et al. (1995, 1997)
Fluctuations of minimum density	−50.0 to +120.0%	−77.4 to +173.2%	
Age distributions	See above	See above	See above

HELMHOLTZ
ZENTRUM FÜR
UMWELTFORSCHUNG
UFZ

Example: Added value of using models



Common shrew model: 20% mortality on April 1 every year

Wang & Grimm (2010).

CAN THIS MODEL BE USED FOR ERA?

- We as scientists belief that this is a fairly good model
- Still difficult to assess by regulators
- Other models still look completely different (matrix, ODE, hypercomplex ABMs)
- What to do?

TRACE’s basic idea

cartoon copyright Kaz Cooke

TRACE

- Independent of
  - **Species or system**
  - **Specific question**
  - **Model type used**
- **Documentation** of model and modelling process **always** follows **the same** terminology and structure

Box 1. TRACE (transparent and comprehensive ecological modeling) documentation structure

I. Model development

Problem formulation: *Context* in which the model will be used, and the type of audience addressed; *specification of the question(s)* that should be answered with the model; statement of the *domain of applicability* of the model, including the extent of acceptable extrapolations; assessment of the *availability of knowledge and data*; specification of necessary *model outputs*.

Design and formulation: Description of the *conceptual model*; description and justification of the *modeling approach* used and of the *complexity*; *entities and processes represented* in the model; most important, the applied *assumptions* about the system.

Model description: Detailed *description of the actual model* and how it has been *implemented* (programs, software platforms, scripts).

Parameterization: *List of all parameter values* used in the model, the *data sources*, and how the parameter values were obtained or calculated; *uncertainties* associated with each parameter.

Calibration: Documentation of the *data sets used* for calibration; *which parameters* were calibrated; what *optimization method* was used.

II. Model testing and analysis

Verification: Assessment of whether the model is working according to its specifications; documentation of what tests have been conducted.

Sensitivity analysis: Exploration of the model behavior for *varying parameters*; documentation of which *parameter combinations* have

AGAIN: WHY NO G.M.P. SO FAR?

- **Lack of inclusion of stakeholders ✓**
- **Inconsistent terminology ✓**
- **Lack of incentives for modellers to follow good practice**

TRACE

- To be used as **„modelling notebook“**
- Just document, on a **daily basis**, what you did using the terminology and structure of TRACE
- From that, generate Appendices for dossiers and scientific publications
- **Incentive for modellers**: organize your work, checklist of important tasks, transparency and comprehensiveness

TRACE

- To be used as a **checklist** for modellers and model users/decision makers
- To be used as a **framework** for developing acceptance criteria:
  - „To accept the model-based risk assessment, validation needs to include…, uncertainty analysis needs to include…, documentation of testing needs to include…“

ROADMAP FOR ESTABLISHING TRACE

- Establish TRACE first
- Then, start using it as a framework for discussing „good modelling practice“ itself

Box 1. TRACE (transparent and comprehensive ecological modeling) documentation structure

I. Model development

Problem formulation: *Context* in which the model will be used, and the type of audience addressed; *specification of the question(s)* that should be answered with the model; statement of the *domain of applicability* of the model, including the extent of acceptable extrapolations; assessment of the *availability of knowledge and data*; specification of necessary *model outputs*.

Design and formulation: Description of the *conceptual model*; description and justification of the *modeling approach* used and of the *complexity*; *entities and processes represented* in the model; most important, the applied *assumptions* about the system.

Model description: Detailed *description of the actual model* and how it has been *implemented* (programs, software platforms, scripts).

Parameterization: *List of all parameter values* used in the model, the *data sources*, and how the parameter values were obtained or calculated; *uncertainties* associated with each parameter.

Calibration: Documentation of the *data sets used* for calibration; *which parameters* were calibrated; what *optimization method* was used.

II. Model testing and analysis

Verification: Assessment of whether the model is working according to its specifications; documentation of what tests have been conducted.

Sensitivity analysis: Exploration of the model behavior for *varying parameters*; documentation of which *parameter combinations* have

FURTHER CREAM APPROACHES

1. **The Modeling Cycle → TRACE**
2. **ODD protocol** for describing IBMs plus extension to other model types
3. **Rigorous model evaluations**, e.g. verification, sensitivity analysis, uncertainty analysis, validation
4. Combining different model types
5. Peer review of model/ling documentations

RIGOROUS MODEL EVALUATIONS

1. Use TRACE as framework and **checklist** for model analysis
2. Document and **communicate** tests and analyses
3. Strive for **structural realism** via **independent**, or secondary, **predictions**:

   Pattern-oriented Modeling

PATTERN-ORIENTED MODELING

1. Provide state variables so that **multiple patterns observed** in reality in principle also can emerge in the model
2. Contrast **alternative sub-models** of certain adaptive behaviours
3. Use multiple patterns to determine entire sets of unknown parameters („**inverse modelling**“)

REVIEW

Pattern-Oriented Modeling of Agent-Based Complex Systems: Lessons from Ecology

Volker Grimm,[1*] Eloy Revilla,[2] Uta Berger,[3] Florian Jeltsch,[4] Wolf M. Mooij,[5] Steven F. Railsback,[6] Hans-Hermann Thulke,[1] Jacob Weiner,[7] Thorsten Wiegand,[1] Donald L. DeAngelis[8]

Agent-based complex systems are dynamic networks of many interacting agents; examples include ecosystems, financial markets, and cities. The search for general principles underlying the internal organization of such systems often uses bottom-up simulation models such as cellular automata and agent-based models. No general framework for designing, testing, and analyzing bottom-up models has yet been established, but recent advances in ecological modeling have come together in a general strategy we call pattern-oriented modeling. This strategy provides a unifying framework for decoding the internal organization of agent-based complex systems and may lead toward unifying algorithmic theories of the relation between adaptive behavior and system complexity.

What makes James Bond an agent? He has a clear goal, he is autonomous in his decisions about achieving the goal, and he adapts these decisions to his rapidly changing situation. We are surrounded by such autonomous, adaptive agents: cells of the immune system, plants, citizens, stock market investors, businesses, etc. The agent-based complex systems (*1*) (ACSs)

Bottom-up models have been developed for many types of ACSs (*4*), but the identification of general principles underlying the organization of ACSs has been hampered by the lack of an explicit strategy for coping with the two main challenges of bottom-up modeling: complexity and uncertainty (*5*, *6*). Consequently, model structure often is chosen ad hoc, and the focus is often on how to

Ecology, in the past 30 years, has produced as many individual-based models as all other disciplines together have produced agent-based models (*13*), and has focused more on bottom-up models that address real systems and problems (*14*).

We describe here how observed patterns can be used to optimize model structure, test and contrast theories for agent behavior, and reduce parameter uncertainty. Finally, we discuss POM as a unifying framework for the science of agent-based complex systems in general.

Patterns for Model Structure: The Medawar Zone

Finding the optimal level of resolution in a bottom-up model's structure is a fundamental problem. If a model is too simple, it neglects essential mechanisms of the real system,

HELMHOLTZ ZENTRUM FÜR UMWELTFORSCHUNG UFZ

SUMMARY

- Ecological risk assessment
- Potential of ecological models
- Aims and scope of CREAM
- The modelling cycle
- Standard documentation format TRACE
- Good modelling practice
- “Well, I should use TRACE…”
- “Well, they might expect TRACE…”

http://cream-itn.eu