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# The concept of stability fields and hot spots in ranking of environmental chemicals

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**Abstract**

In contrast to conventional multi-criteria decision aids, such as the well known PROMETHEE approach, AHP or the different versions of ELECTRE, we support the basic assumption of environmetrics: let first the data speak, and then let us include subjective preferences in order to get a unique decision. In the present paper we introduce and discuss the decision support system METEOR (Method of Evaluation by Order Theory). The basis of the method is a data matrix. The rows are defined by the objects which are to be evaluated; the columns are defined by the attributes, which characterize the objects with respect to the evaluation problem. By means of the attributes a partial order is derived. In subsequent steps attributes are aggregated by a weighting procedure, allowing a high degree of participation of stakeholders and other participants of the planning process. The aim is to enrich the partial order stepwise, until the objects of interest can be compared. The software WHASSE written in Delphi is available for scientific purposes from the first author.

As an example we evaluate 12 high production volume chemicals (HPVC) which have been detected in the environment by four attributes and discuss the enriched partial order after introducing some weights. It turns out that in some cases the weights have almost no influence concerning the evaluation result, whereas in some other cases slight variations of weights drastically change the evaluation result. Therefore, the metric space spanned by weights can be partitioned in so-called ''stability fields'' where the evaluation result is invariant and in so-called ''hot spots'', where the evaluation is strongly changing. This characterisation of the space of weights is helpful for stakeholders to express their preferences.


*Keywords:* HPV chemicals; Environmental chemicals; Ranking; Posets; Hasse diagram technique (HDT); Decision support systems; Cluster analysis; Method of Evaluation by Order Theory (METEOR); Stability fields; Environmetrics; Environmental software

## 1. Introduction

Multi-criteria decision making becomes more and more important in environmental sciences and hence quite a few research projects focus on this topic. For example the MULINO Decision Support System (mDSS) has been developed for implementing the European Water Framework Directive, namely integrating environmental, social and economic concerns (Giupponi, 2007). Another example concerning the Integrated Water Resources Management (IWRM), is a multi Objective Decision Support System (MODSS) which has been developed and applied to the planning of the Lake Maggiore (Castelletti and Soncini-Sessa, 2006). The Elbe-Decision Support System is a computer based system for integrated river basin management of the German river Elbe basin and is therefore another example for an environmental decision

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support system (Berlekamp et al., 2007). A methodology based on a hybrid approach that combines fuzzy inference systems and artificial neural networks has been used to classify the ecological status in surface waters. This methodology is applied to sampling sites in the Ebro river basin and can support decision makers in evaluation and classification of ecological status, as required by the EU Water Framework Directive (Ocampo-Duque et al., 2007). The chemical speciation model BIOCHEM comprises ecotoxicological transfer functions for uptake of metals (As, Cd, Cu, Ni, Pb, and Zn) by plants and soil invertebrates and is another example for a flexible and dynamic decision support system (DSS) to analyse natural or anthropogenic changes that occur in river systems (Vink and Meeussen, 2007). A further interesting work including the spatial factor is a multi-criteria decision making approach applied to urban water management (Makropoulos and Butler, 2006). Concepts for the use of techniques of decision analysis to structure scientist and stakeholder involvement in river rehabilitation decisions are published by Reichert et al. (2007). The software, named proDEX is also applied as a multi-criteria decision support model in environmental sciences (Znidarsic et al., 2006).

Decisions concerning risk assessment of chemicals are to be supported by information about exposure and effects of chemicals. Both, exposure and effects are used as attributes/indicators to evaluate the chemicals under investigation. For the subsequent evaluation of chemicals, many methodological approaches are available, requiring in principle the same working steps, which are discussed in more detail in Simon et al. (2005) and Klauer et al. (2001). One step, namely the evaluation algorithm is often almost disregarded in real evaluations. The chosen evaluation approach however influences the evaluation result and the participation of stakeholders. The efficiency of participation of stakeholders and the acceptance of the decision result in turn depends on the transparency of the evaluation procedure. For example: decisions about complex problems such as chemical risk assessment will include conflicting attributes. To solve such conflicts, the most commonly used approaches include the methodological step of attributes' aggregation. The benefit of the aggregation step is that finally a linear ranking of the objects (here: chemicals) can be obtained, identifying *one* best solution, e.g. the chemical with the lowest risk. Aggregation often implies a trade off among attributes: a bad evaluation in one or more attribute(s) can be compensated for by a good evaluation in other attributes. However, attributes can represent fundamentally different aspects such as accumulation, mobility and toxicity. Therefore the methodological idea followed in this paper is to take first a purely statistical explorative point of view (i.e. "let first the data speak") and to include additional knowledge, e.g. the preferences of the stakeholder, in separate steps in order to keep a maximal control over the effect of including additional knowledge.

The paper is organized as follows: in Section 2 the example of 12 high-production volume chemicals (HPVC) is introduced, the methods Hasse diagram technique (HDT) and Method of Evaluation by Order Theory (METEOR) and the concept of crucial weights together with their analysis toward the introduction of "*g*-spectra, stability fields and hot spots" are explained. Whereas for the sake of demonstration a simpler example is used, Section 3 shows the application of METEOR on the HPVC data matrix. A detailed discussion about possible extensions of the method concludes the paper. Additionally, there are appendices 1–4, where abbreviations, symbols and concepts are listed (Appendix 1) and where some counting formulas are explained (Appendices 2–4).

## 2. Materials and methods

### 2.1. Data preprocessing

With publication of the White Book of the EU (EEC, 2001) and of the REACH-procedure (European Commission, 2006) the interest in ranking of chemicals as a preparatory step is renewed: here the data matrix (12 high production volume chemicals) define the rows, and 4 attributes define the columns), first published by Lerche (2002a) is taken as a ranking example and is more extensively described in the Section 3. We are calling the set of objects (i.e. of chemicals) C.

"Results". Note, that we refer to 'objects' instead of chemicals as long we are not discussing the real life example.

Often it is necessary to transform a data matrix into the appropriate form i.e. into the closed interval [0,1] for an evaluation:

(i) a normalization by

$$\overline{q}_i(j) := \frac{q_i(j) - q_i(\min)}{q_i(\max) - q_i(\min)}, \quad i = 1, \ldots, 4, \quad j \in C$$

(ii) check for a common orientation (high numerical value indicates a high risk) by multiplying attributes − if necessary − with −1 or another appropriate transformation

(iii) shifting negative values to positive entries by adding a positive number to the attribute values.

The subjective preferences of stakeholders are expressed by weights, which are taken from the closed interval [0,1]. We consider the weights as 'external knowledge', whereas the data matrix expresses the basic information taken from measurements or modelling.

### 2.2. Hasse diagram technique

Several well-known evaluation algorithms are available such as PROMETHEE (Brans and Vincke, 1985), AHP (Saaty, 1994), MAUT (Schneeweiss, 1991), ELECTRE (Roy, 1990) or NAIADE (Matarazzo and Munda, 2001). All these methods include an aggregation of attributes by including subjective preferences and therefore cannot be considered as purely data explorative methods. Beyond this it is difficult to trace back how the evaluation result was influenced by parameters to run those algorithms. Hence we consider these high sophisticated methods on the one side as efficient, as they deliver a unique decision, but on the other side as not transparent and difficult to handle as all preferences must be at hand simultaneously.

An alternative approach is provided by simple elements of partial order theory, such as Hasse diagram technique (HDT) (Brüggemann and Voigt, 1995; Brüggemann and Welzl, 2002; Brüggemann and Carlsen, 2006; Brüggemann et al., 1994, 2001, 2006a; Voigt et al., 2004a,b, 2006). For the sake of clarity we define some important concepts used in this paper.

Definition 1. We call $x$ an object and C the ground set that is the set of objects.

Definition 2. $q_i(x)$ is the $i$th attribute of the object $x$ and $IB = \{q_i | i = 1, 2, \ldots, m\}$ the set of m attributes (information base).

Definition 3. Let $x, y \in C$ and $q_i \in IB$, then $x \leq y$ if $q_i(x) \leq q_i(y)$ for all $i = 1, 2, \ldots, m$. We say that $x$ and $y$ are comparable. If the orientation does not play a role, we write $x \perp y$ to express that $x$ and $y$ are comparable.

By definition 3 a product- (or component-wise-) order is given and it obeys the following axioms of order:

(i) reflexivity (an object can be compared with itself)
(ii) antisymmetry (if an object $x$ is better that $y$, then $y$ is worse than $x$)
(iii) transitivity (if $x, y, z \in C$ and $x \leq y$ and $y \leq z$ then $x \leq z$).

Definition 4. Two objects $x, y \in C$ are called incomparable ($x||y$) if there is at least one $q_i$ with $q_i(x) > q_i(y)$ and one $q_j$ with $q_j(x) < q_j(y)$.

Sometimes we add further information to the order relation. For example $b||_{q1,q2}d$ expressing that $b$ is incomparable with $d$ with respect to the attribute values of $q_1$ and $q_2$. The evaluation result, a partially ordered set, is visualized in a Hasse diagram (HD) (see e.g. Fig. 1). We show in Table 1 an example of a data matrix used to evaluate a set of 5 objects $C = \{a, b, c, d, e\}$ characterized by two attributes ($q_1$ and $q_2$).

Hasse diagrams are digraphs, which have no cycles (because of the order-axiom of antisymmetry) and – as ordinary graphs – have no triangles (because of the order-axiom of transitivity). The software realization of HDT, "WHASSE" (Brüggemann et al., 1999) provides several tools for convenient and detailed data analysis such as the sensitivity of the structure of the digraph with respect to different attributes (Brüggemann et al., 2001; Brüggemann and Welzl, 2002). The software is available for scientific purposes from the first author. WHASSE is written in Delphi, equipped with a comfortable GUI running under the operation system Windows NT and XP. As no compensation among attributes is carried out at all, conflicting evaluations of attributes cannot be methodologically removed. Consequently multiple favourable objects can be identified as incomparable winners. In our example (Table 1, Fig. 1) assuming that low values are favourable there are two incomparable objects, namely $a$ and $c$. Altogether we find three incomparabilities in the Hasse diagram, symbolically written as: $b||d$, $b||c$ and $a||c$ and five cover-relations denoted by the symbol "$\cdot>$" and lines in Fig. 1, (details, see Brüggemann et al., 1994) $e\cdot > b$, $e\cdot > d$, $b\cdot > a$, $d\cdot > a$ and $d\cdot > c$.

## 2.3. A new concept to solve the problem of incomparable objects: METEOR

### 2.3.1. Overview

Partial order theory provides many concepts to derive linear orders without any additional introduction of (stakeholder's) preferences (Lerche et al., 2002b, 2003; De Loof et al., 2006). As no subjective weighting is involved the linear order obtained from a partial order is called a "canonical (linear) order" (Brüggemann et al., 2004, 2005). In contrast to derive canonical linear orders, METEOR (Method of Evaluation by Order Theory) attempts to resolve the incomparabilities among objects by inclusion of external knowledge. METEOR intends to obtain a clear decision (one best object), maintaining transparency and allowing participation [see for details Simon et al. (2005) and Voigt and Brüggemann (2005)]. It is conceptually based on the well known and often used concept of a hierarchy of criteria in multi-criteria decision aids (as e.g. in the AHP method (Saaty, 1994)). Basically METEOR allows a step-by-step aggregation of attributes by forming e.g. weighted sums about subsets of attributes. Principally non-linear aggregation (non-linear with respect to attributes) is also possible but still has not worked out because of its inherent complexity.

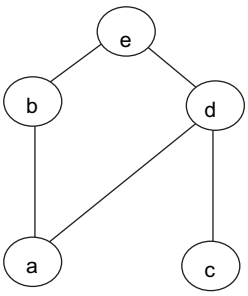


Fig. 1. Hasse diagram of the data matrix of Table 1.

Table 1
Data matrix as an example to construct a Hasse diagram (Fig. 1)

| Objects | $q_1$ | $q_2$ |
|---|---|---|
| $a$ | 15 | 5 |
| $b$ | 25 | 35 |
| $c$ | 10 | 60 |
| $d$ | 20 | 70 |
| $e$ | 60 | 80 |

The possibility of a step-by-step aggregation of attributes provides the freedom to thoroughly analyse the effects of attribute weights and compensation. Furthermore, preferences (attribute weights) which are most sensitive to the evaluation result can easily be identified.

One may consider the data matrix characterizing the objects by attributes as primary knowledge, which is based on measurements, mathematical models, causal relations. Inclusion of knowledge beyond the data matrix means that relations are supposed among the attributes and implies external information: for example, one may consider one attribute to be more important than another one (Brüggemann et al., 2006b). Here we introduce the notion of "importance" of attributes from a technical, pragmatic point of view: importance is expressed by weights. In Fig. 2 HDT, METEOR and conventional algorithms like PROMETHEE, ELECTRE, etc. are compared: it is schematically shown how the inclusion of weights (external knowledge) reduces the transparency and the objectivity of the decision process (dashed line), whereas the efficiency (i.e. the ability to identify uniquely a best (or worst) object) of the decision process (continuous line) is enhanced. Methods, such as HDT may be located at the high transparency and low efficiency side, and methods like PROMETHEE at the high efficiency and low transparency side. METEOR may be located in between these two extreme cases.

### 2.3.2. METEOR as iterative application of HDT

The kernel of METEOR is the Hasse diagram technique (HDT). METEOR is discussed in detail by Simon et al. (2005) and was developed to solve conflicts among objects stepwise. Taking a look at two objects $x$, $y$ characterized by m attributes it often occurs that one of them is evaluated better in one attribute and worse in the other one and the other way round. The incomparabilities $x||y$ between any two objects indicate the conflict among at least two of their attributes and one may decide that compensation is useful. Then a new "aggregated attribute", for example by a weighted sum of two original attributes may be constructed. The new information base IB' consists now instead of originally $m$ attributes of only $m$-1 and the number of comparabilities increases. If the aggregation is done in such a way that a weak positive monotonous function $f$ of attributes is found, then this aggregation is equivalent with

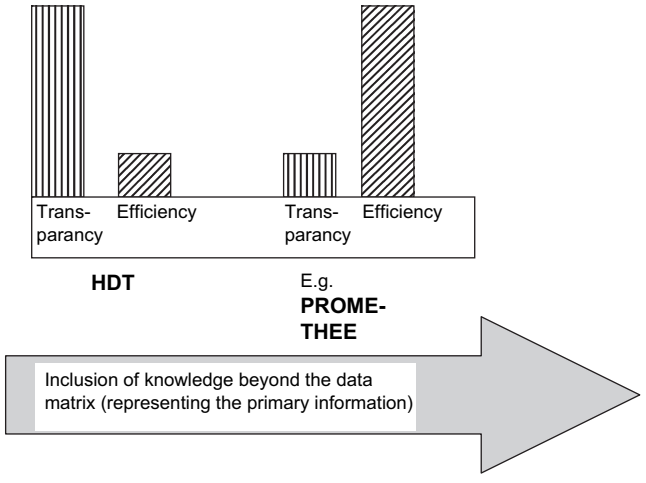


Fig. 2. Behaviour of transparency, objectivity and efficiency of a decision process (see text for further explanation).

an order preserving map. Presently in METEOR specifically a linear function is selected, however, non-linear aggregations are not excluded but more difficult to evaluate by explicit analytical expressions (see later). The step-by-step aggregation can be carried out until one single "aggregated hyper-attribute" is obtained, which is considered as a weighted sum of all original $m$ attributes, and which will lead to a linear ranking of all objects (in technical terms: a weak linear order (because equivalent objects may appear)).

*2.3.3. Aggregation strategies*

If m attributes are considered then basically $2^m$-$m$-2 attribute subsets can be potential candidates for forming new aggregated attributes (see Appendix 2). It is hypothesized that it is not meaningful to include subsets which are not disjoint, hence a more suitable base to discuss the stepwise aggregation is to analyze the partitions of IB (Appendix 3). It is well known that the number of partitions one can obtain, can be calculated after the Stirling numbers of the second kind if the number of classes is known (Appendix 4) (see for example Brüggemann and Drescher-Kaden, 2003, p. 95 f) or – if the number of classes is left open – by the Bell formula (Appendix 5) (Bock, 1974). Taking for example four attributes and assuming two classes for the partitioning, we get 7 partitions (one of these, for example, is $\{(q_1, q_2), (q_3, q_4)\}$ another one $\{(q_1, q_2, q_3), (q_4)\}$).

If, for example, 20 attributes are considered, then by applying the Bell formula $10^{13}$ partitions are possible, i.e. $10^{13}$ disjoint subsets of attributes can be formed in order to aggregate the attributes. Therefore some kind of heuristics is needed to find a way through the jungle of possible aggregations.

Clearly from a logical point of view one should start with attributes belonging to one sub-criterion. If for example chemicals are to be evaluated, one may consider exposure attributes on one side as candidates for an aggregation and effect attributes as candidates for another aggregation, obtaining two super-attributes "Exposure" and "Effects". This point of view is comfortable for stakeholders as it allows them first to consider general aspects and then – perhaps – to go into details. We had in mind this procedure, when we first established METEOR. From the point of evaluation we might call this procedure a *bottom-up procedure* (from the basis of detailed information, to more generalized concepts via sub-criteria). However similar attributes are often well correlated (indeed one may even define similarity by the correlation behaviour) and their aggregation has little effect on the poset and is consequently of little use for decision making. More efficient is to aggregate those attributes which have a high degree of conflicting potential. Those attributes are often anti-correlated. Hence their aggregation will rather efficiently reduce the incomparabilities. This kind of procedure one may call a *top-down procedure*: first reduce the most conflicting attribute subsets and then analyze the results by applying partial order. Even if we have decided which procedure we will follow it is not clear how the aggregation functions should look like (linear or non-linear). Before we proceed, some more definitions and notations are needed:

Definition 5. We call $S(k) = \{q_i | i < m\}$ the set of aggregated attributes and $n(k)$ its cardinality.

The corresponding super-attribute, $\varphi_k$ based on $S(k)$, is calculated as

$$\varphi_k = \sum_{i=1}^{n(k)} g_i q_i$$

together with the normalization:

$$\sum_{i=1}^{n(k)} g_i = 1 \quad \text{and} \quad q_i \in S(k).$$

If we call $n(k) < m$ the number of attributes actually aggregated, then any super-attribute has (because of the weights' normalisation) $n(k) - 1$ "freedom" of freely varying the scalars $g_i \in [0,1]$. We call $[0,1]^{n(k)-1}$ the $g$-space of the $k$th super-attribute. Therefore we associate to any super-attribute a metric space of weights with the dimension $n(k) - 1$ and any aggregation step in METEOR is accompanied by the product of all $g$-spaces, which we call the $G$-space. In general $n(k)$ may vary and may depend on the intuition of the researcher, applying METEOR. Here, however, we restrict ourselves on aggregation schemes with freedom 1, i.e. we analyze in the subsequent parts of the paper for any super-attribute a $g$-space of dimension 1. If we combine for example

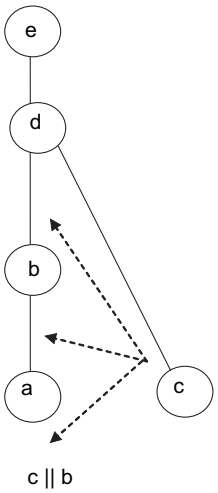


Fig. 3. Scheme explaining the "local" condition derived from $c||b$. For object $c$ above $b$ there is only one accessible position; for $c$ below $b$ there are two positions available.

(as we will do and describe later) four attributes pairwise to two super-attributes, the two linear $g$-spaces are combined, forming a two-dimensional space $[0,1] \times [0,1]$. As we also will see later in the text, the restriction to freedom = 1 simplifies considerably the procedure and we call a procedure, based on a purely pairwise combination of attributes the "orthogonal-METEOR" (abbr.: o-METEOR). In another paper Restrepo et al. describe a non-orthogonal METEOR procedure, with refrigerants as an example (Restrepo et al., 2007a).

Finally – depending on the task of the decision procedure – a good idea is not to perform aggregations until a linear order is generated, but to stop the aggregation if at least a greatest or a least element is found or if any two objects of specific interest can be compared. We call this strategy the "*extremal case – procedure*".

Careful analysis is needed if attributes which will be combined by a weighted sum are not on the same scaling level, if for example continuous variables are used in the evaluation process together with linguistic ones, even if one gives them an ordinal or metric interpretation. The best strategy in such cases is, just to stop the aggregation process before attributes of different scaling levels are numerically combined. We see the possibility of taking care of different scaling levels as a main advantage of the step-wise procedure in METEOR. Here, however for the sake of demonstration the role and structure of $g$-spaces we consider all attributes as metric quantities.

## 2.4. The concept of crucial weights

Imagine that four attributes, i.e. IB = $\{q_1, q_2, q_3, q_4\}$ are pairwise aggregated as follows:

$$\varphi_1 = g_1 * q_1 + (1 - g_1) * q_2 \tag{1a}$$

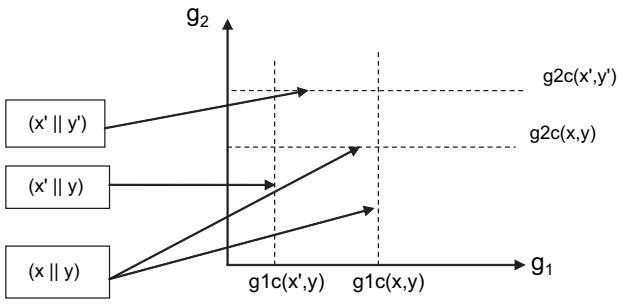


Fig. 4. Exemplifying conclusion 7 in the case of two dimensions (i.e. aggregating attributes pairwise to two super-attributes).

Table 2
Towards $H_k$: if there are two attributes gathered in $k$ then for each pair of objects one has to calculate $\Delta_i$, $Q$ and gkc

| $k$ index | Pair | $\Delta_1$ | $\Delta_2$ | $Q$ | gc |
|---|---|---|---|---|---|
| 1 | ac | $15-10=5$ | $5-60=-55$ | $-0.09$ | 0.917 |
| 2 | bc | $25-10=15$ | $35-60=-25$ | $-0.6$ | 0.625 |
| 3 | bd | $25-20=5$ | $35-70=-35$ | $-0.143$ | 0.875 |

$H_1(0.917)=1$, $H_2(0.625)=1$, $H_3(0.875)=1$.

and

$$\varphi_2 = g_2 * q_3 + (1-g_2) * q_4 \tag{1b}$$

Now, assume that the object $x \in C$ is incomparable with object $y$ due to:

$$q_1(x) > q_1(y) \quad \text{and} \quad q_2(x) < q_2(y).$$

For this case we write: $x||_{q1,q2}y$.

If $x||_{q1,q2}y$ then the result of aggregation (1a) for those particular objects $x$ and $y$ depends on the weight $g_1$. Obviously the equation

$$\varphi_1(x) = \varphi_1(y) \tag{2}$$

determines the $g_1$ value where the character of order relation between $x$ and $y$ changes. Note firstly that Eq. (2) is the reason that non-linear aggregation functions will be more difficult to evaluate: instead of an analytical expression derived from Eq. (2) a numerical procedure maybe needed. Secondly, note that Eq. (2) is a "local" condition regarding $x$ and $y$, as it only determines $x > y$ or $x < y$ but not necessarily the actual order relationships of all objects from C. A scheme (Fig. 3) may be useful for a better understanding.

Eq. (2) determines the transition from $x < y$ to $x > y$ but not the final position or the final resulting configuration. The number of all configurations is less than $2^U$, with $U$ the number of incomparable pairs. A correct application of Eq. (2) has to regard all incomparable pairs and the final configuration must be constructed from all possible outcomes under the constraints of transitivity (see below).

After introducing

$$\Delta_i^{x,y} := q_i(x) - q_i(y) \tag{3a}$$

and

$$Q_{ij}^{x,y} := \frac{\Delta_i^{x,y}}{\Delta_j^{x,y}}. \tag{3b}$$

we find because of the supposed linearity of the aggregation function from Eq. (2):

$$g_1^c(x,y) = \frac{\Delta_2^{x,y}}{\Delta_2^{x,y} - \Delta_1^{x,y}} \tag{4a}$$

or

$$g_1^c(x,y) = \frac{1}{1 - Q_{1,2}^{x,y}}. \tag{4b}$$

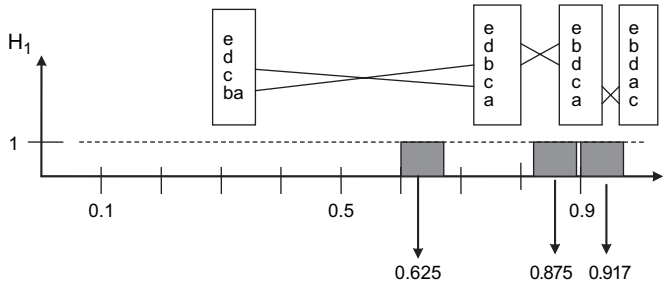


Fig. 5. $g$-spectrum derived from the data matrix of Table 1.

Table 3
Signs of $\Delta_i$ and their possible role if a boundary of a stability field is passed

| Case | $\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ | "Reaction" $g_1$ small[1)] → large[1)] |
|---|---|---|---|---|---|
| 1 | + | − | + | + | $x\|\|_{\varphi1,\varphi2}y \rightarrow x >_{\varphi1,\varphi2}y$ |
| 2 | + | − | − | − | $x <_{\varphi1,\varphi2}y \rightarrow x\|\|_{\varphi1,\varphi2}y$ |
| 3 | + | − | 0 | + | $x\|\|_{\varphi1,\varphi2}y \rightarrow x >_{\varphi1,\varphi2}y$ |
| 4 | + | − | 0 | − | $x <_{\varphi1,\varphi2}y \rightarrow x\|\|_{\varphi1,\varphi2}y$ |
| 5 | + | − | 0 | 0 | $x <_{\varphi1,\varphi2}y \rightarrow x >_{\varphi1,\varphi2}y$ |

One pair $(x, y)$ is assumed and $\Delta_i = q_i(x) - q_i(y)$.

To simplify the notation we also write gkc if just "crucial weights" are mentioned and $g(k)$ $(x, y)$ (omitting the index "$c$" for "crucial") if we relate to the subset $S_k$ and the objects $x$ and $y$.

There are some observations, namely that

1. Crucial values for the weights depend on the pair of objects, whose order relation is to be examined.
2. Crucial weights have only values within the closed interval [0,1] if Q is $\leq 0$. If $x$, $y$ are comparable, $Q$ becomes a positive number and the crucial weight would get values larger than 1. Therefore
3. Eqs. (4a) or (4b) is only meaningful if we discuss incomparable objects.
4. As all incomparable pairs are to be taken into account the set of all crucial weights is important if o-METEOR is to be applied.
5. In o-METEOR the crucial weight of two objects does not depend on the values of other weights. Hence in the product-space of weights, the G-space, each condition of type (4) defines parallel or orthogonal (hyper-) planes. (If only two super-attributes are formed we obtain parallel or orthogonal lines in the $g_1$, $g_2$-positive orthant).
6. It is possible that several pairs $(x, y)$, $(x', y')$, $\ldots \in C \times C$ have the same gkc-values. This is especially the case if the data matrix consists of integers. Hence it is of interest to count the pairs belonging to one numerical value of gkc. The count is summarized by the $H_k(\,g(k)^c$ function (see the next section, Eq. (7)).
7. One pair $(x, y)$ can only have exactly one gkc-value for a fixed aggregation of the selected attributes in the set $S_k$. If different attributes are aggregated and the same pair $(x, y)$ is considered, then it can be build a set of {g1c, g2c, …} in the $G$-space gathering particular gkc for those particular aggregations. In that latter case one pair must have an intersection of several (hyper-) planes. A scheme (Fig. 4) may be helpful to explain this.

In Fig. 4 it is assumed that the incomparabilities of $(x', y')$ and $(x, y)$ resp. are associated with crucial weights for $\varphi_2$ (Eq. (1b)). In contrast, the incomparability of $(x', y)$ is related to $\varphi_1$ (Eq. (1a)). Note that in Fig. 4 the pair $(x, y)$ has two crucial weights, which necessarily must be assigned to different $g$-spaces, i.e. to $\varphi_1$ and to $\varphi_2$.

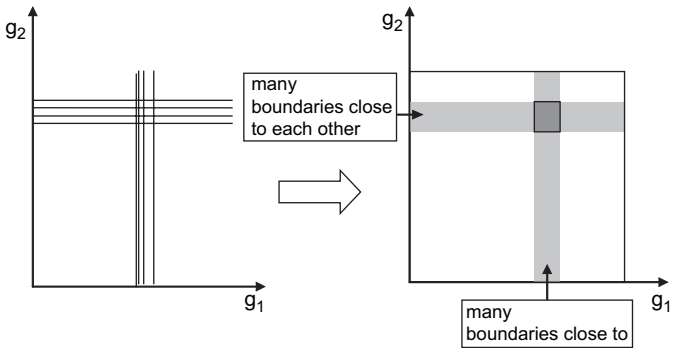


Fig. 6. Instead of a single line several single lines may appear which are close to each other. A hot spot in the $G$-space at the intersection points (dark rectangle).

Table 4
Primary information

| Name and abbr. | PV: production volume as score | LC50: Acute fish toxicity [mg/L] | Log Kow | BD: [% degradation/ day] |
|---|---|---|---|---|
| 1-chloro-nitrobenzene (CNB) | 4 | 1.5 | 2.6 | 0.2 |
| 4-nitroaniline (4NA) | 2 | 35 | 1.4 | 0 |
| 4-nitrophenol (4NP) | 1 | 7 | 1.9 | 0.1 |
| Atrazin (ATR) | 2 | 4.3 | 2.5 | 0.5 |
| Chlormequat chloride (CHL) | 2 | 80 | −2.2 | 1 |
| Diazinon (DIA) | 1 | 2.6 | 3.3 | 0 |
| Dimethoate (DIM) | 2 | 7.5 | 0.7 | 0 |
| Ethofumesate (LIN or ETH) | 1 | 11 | 2.7 | 0.4 |
| Glyphosphate (GLY) | 2 | 52 | 0.002 | 0.3 |
| Isoproturon (ISO) | 2 | 3 | 2.5 | 30 |
| Malathion (MAL) | 3 | 0.04 | 2.7 | 100 |
| Thiram (THI) | 2 | 0.3 | 1.7 | 0 |

Here it may be a good place to demonstrate the role of Eqs. (2) and (3) by revisiting Fig. 3. In Fig. 3 there are two incomparabilities ($c \,||\, a$) and ($c \,||\, b$). Hence in general we will obtain two crucial weights ${g_1}^c$ ($b$, $c$) and ${g_1}^c$ ($a$, $c$) (if the simplest case of two attributes is supposed). Starting with the equation for ($c \,||\, b$) it depends on the selected value for the weight whether $c > b$ and hence $c > a$, or $c < b$ is obtained. If $c < b$ is found, we need another information, namely resulting from the Eq. (2) for ($a \,||\, c$). The outcome is once again twofold: $c > a$ or $c < a$, therefore two inequalities imply two equations of type (2), four possible orders for ($c$, $b$) and ($c$, $a$) resp., but only three final configurations.

### 2.5. Stability fields and hot spots

It is oversimplified to consider that any pairwise aggregation leads to a well separated set of $g_k^c$-values. An example of well separated parallel, orthogonal gkc-values can be found in Brüggemann et al. (2006b) (here also an example of non-orthogonal METEOR was given). In order to pave the way of handling the case of many gkc-values, we introduce some further concepts:

If $m$ attributes are pairwise aggregated and those aggregations are disjoint then the $G$-space has the dimension $p$.

$$p := \begin{cases} m/2 & \text{if} \quad m = 2*n, \quad n = 1, 2, 3, \ldots \\ (m-1)/2 & \text{if} \quad m = 2*n+1, \quad n = 1, 2, 3, \ldots \end{cases} \tag{5}$$

The calculation of gkc values refers to pairs of objects $x$, $y$ which are incomparable (see Eq. (2) in Section 2.4). Hence sets of pairs $x||_{qi,qj}y$ play a basic role. Then we call

Table 5
After normalization, orientation and shifting of the data

| Chem | PV | LC | Log Kow | BD |
|---|---|---|---|---|
| CNB | 1 | 0.98 | 0.87 | 1 |
| 4NA | 0.33 | 0.56 | 0.65 | 1 |
| 4NP | 0 | 0.91 | 0.74 | 1 |
| ATR | 0.33 | 0.95 | 0.85 | 1 |
| CHL | 0.33 | 0 | 0 | 0.99 |
| DIA | 0 | 0.97 | 1 | 1 |
| DIM | 0.33 | 0.91 | 0.53 | 1 |
| LIN | 0 | 0.86 | 0.89 | 1 |
| GLY | 0.33 | 0.35 | 0.40 | 1 |
| ISO | 0.33 | 0.96 | 0.85 | 0.7 |
| MAL | 0.67 | 1 | 0.89 | 0 |
| THI | 0.33 | 1 | 0.71 | 1 |

Table 6
Pearson correlation matrix

| | PV | LC | Log Kow |
|---|---|---|---|
| LC | 0.074 | | |
| Log Kow | 0.000 | 0.896 | |
| BD | −0.364 | −0.251 | −0.258 |

$$\mathrm{IC}_k := \{(x,y) | x, y \in \mathrm{C}, x||_{q_i,q_j} y, q_i, \; q_j \quad \text{belong to set } k\} \tag{6}$$

the set of incomparable objects given the pairwise aggregation $k$. As we mentioned above, we indexed $k$ by 1, 2, …, $p$.

Any pair $(x, y) \in \mathrm{IC}_k$ has exactly one gkc if $S_k$ is held fixed (linearity of the aggregation and conclusion 7). However one value of a crucial weight may represent several pairs like ($x$, $y$), ($x'$, $y'$) (Fig. 4). The set of gkc-values in any single $g$-space can be ordered and we call

$$H_k(g(k)) := |\{(x,y) \in \mathrm{IC}_k \text{ having the same gkc} - \text{value}\}| \tag{7}$$

the "$g(k)$-spectrum". $H_k$ is a function operating on the gkc-values of the $k$th $g$-space.

In more technical terms: for the pairs $(x||y) \in \mathrm{C} \times \mathrm{C}$ an equivalence relation $\mathrm{R}(k)$ is introduced as follows:

$$(x||y)\mathrm{R}(k)(x'||y') : \Leftrightarrow g(k)(x,y) = g(k)(x',y'), \quad k - \text{fixed} \in \{1,2,\ldots,p\} \tag{8}$$

Hence given the set $\{(x||y)\} \subset \mathrm{C} \times \mathrm{C}$, then this set is partitioned into $k$-equivalence classes. Each equivalence class is characterized by one and only one gkc-value. Correspondingly $H_\mathrm{k}(g(k))$ counts the elements of any of the $k$-equivalence classes and orders them for increasing values of gkc along the $g$-axis.

Example: we take the data of Table 1, then the dimension of the $g$-space $= p = 1$. $\mathrm{IC}_1 = \{(b, d), (b, c), (a, c)\}$. In Table 2 the calculation is performed.

Hence formally we can draw a spectrum, as shown in Fig. 5.

Performing the aggregation means that we discuss the order relation as a function of $g_1$. Clearly $g_1 = 0$ is a projection onto $q_2$, hence a linear order results: $a < b < c < d < e$. As long as $g_1$ is less than 0.625 there will be no change. Passing this value a change occurs, which refers to the pair ($b$, $c$). The next change in the order relation refers to 0.875, which is assigned to the pair ($b$, $d$), finally a change happens when $g_1$ passes the value 0.917, which is assigned to the pair ($a$, $c$). The resulting four linear orders are found in Fig. 5 too. Theoretically five linear orders are possible, however by checking Eq. (2) only four linear orders are obtained. The configuration $e > d > b > a > c$ which is compatible with the partial order shown in Fig. 1 is not obtained (for more details, see Section 4). In order to introduce the concept of stability fields we define.

Definition 6. The $G$-space is generated by the space of all the weights coming from different aggregations.

Definition 7: Let C be a non-empty object set and IB a set of attributes. The weighted pairwise aggregation of attributes in IB implies that the order relationships of the objects in C change or not, depending on the weights $g$ selected. We call a "stability field" those regions in the $G$-space where the

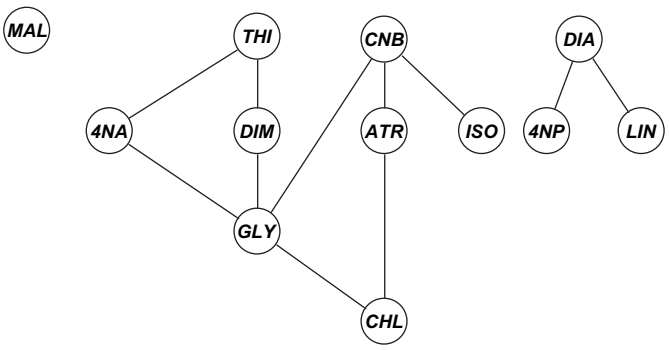


Fig. 7. Hasse diagram (C, IB), $C = \{\mathrm{ATR}, \ldots,\}$, $\mathrm{IB} = \{\mathrm{PV}, \mathrm{LC50}, \text{log Kow}, \mathrm{BD}\}$.

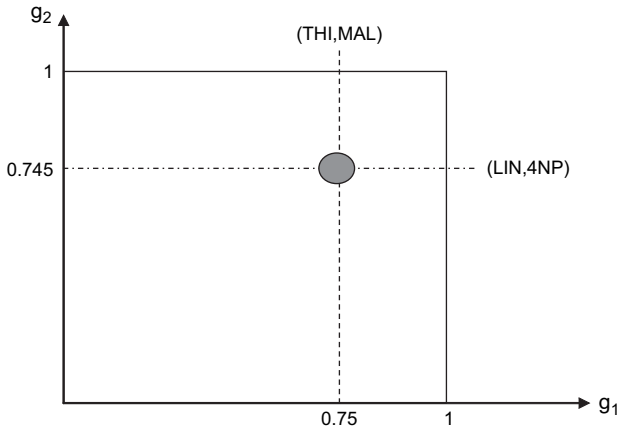


Fig. 8. Two-dimensional *G*-space, and stability fields and hot spots (grey circle).

changes of the weights of aggregation do not change the order relationships of the crucial object-pairs in $IC_1$, $IC_2$, …, $IC_p$.

Definition 8: Stability fields are separated by linear spaces of lower dimensions. In a two-dimensional *G*-space the separating spaces are just lines. The separating linear spaces and their intersections are called "hot spots".

In simple words: hot spots are the regions in the *G*-space where transition from one configuration into another appear; stability fields are those regions in the *G*-space where the configuration of the poset is invariant. In the next sections this is discussed in more detail.

### 2.6. Change of order relations at crucial g-subspaces

As it was shown in (4) the crucial weights depends on the Δ-values found for all pairs of objects which are incomparable if the original IB is applied.

From the example of Table 3 we deduce that each boundary is to be discussed with respect to

- the pairs of objects belonging to this boundary;
- the reactions (in terms of Table 3) related to each of the $(x, y)$-pairs.

### 2.7. Stripes at hot spots as small regions in the G-space

Up to now we discussed some few and well separated gkc-values. If there are $N$ objects then the upper bound for $|IC_k|$ is $N^*(N-1)/2$. Even if $p = 2$ we have to discuss many gkc-values in $g_1$- and in $g_2$-direction, corresponding to $IC_k$. Hence instead of having discrete lines in the *G*-space it may be more convenient to group the lines to stripes as it is shown in Fig. 6.

Therefore it is of primary importance to generalize the concept of the *g*-spectrum: instead of a discrete distribution as formalized by $H_k(g(k))$ (Eq. (7)) one may discuss a quasi-continuous one. A cluster analysis applied to all the gkc-values seems to be the appropriate statistical tool: let us imagine that we consider a clustering for each *g*-space in the o-METEOR on a high similarity level, then a cluster may contain some pairs $\in IC_k$ and each of the pairs is characterized by its gkc-value. Selecting a cluster an interval of gkc-values can be found. Each interval defines a *stripe*. Instead of discrete lines representing discrete gkc-values *transition zones* (consisting of a series of lines close to each other) appear where a small variation of a weight will change the order relations of many $(x, y)$-pairs. Between the stripes there may be rectangular areas in the *G*-space where the position of originally incomparable objects does not change if weights are varied. Therefore these areas (or hypercubes if $p > 2$) are called as before *stability fields*. Furthermore the bundle of hot spots is no more a bundle of linear spaces of a low dimension but may get as a whole a measure $\neq 0$ in the *G*-space. Nevertheless we call the area defined by a bundle of gkc-values as a whole a "hot spot".

## 3. Results

### 3.1. The chemicals

In Table 4 the twelve chemicals are listed up, the attributes are briefly described and the entries are shown. More information about these chemicals, background information to the selection criteria can be found in Lerche et al. (2002b).

### 3.2. Preprocessing of the data and aggregation

As discussed in Section 2 the data matrix (Table 4) needs several preprocessing steps. The final resulting matrix is shown in Table 5.

The Pearson correlation matrix is shown in Table 6; and we start with those two attributes, which have the highest degree of anti-correlation, that are BD and PV and combine the remaining other two attributes, namely LC50 and log Kow. As the leading principle is to find out the highest degree of anti-correlation which dictates the kind of aggregation, we consider this as a top-down-procedure.

$$\varphi_1 = g_1{}^*\mathrm{PV} + (1 - g_1)^*\mathrm{BD}$$

$$\varphi_2 = g_2{}^*\mathrm{LC50} + (1 - g_2)^*\log \mathrm{Kow}$$

In the first example we discuss two pairs of chemicals out of Table 6.

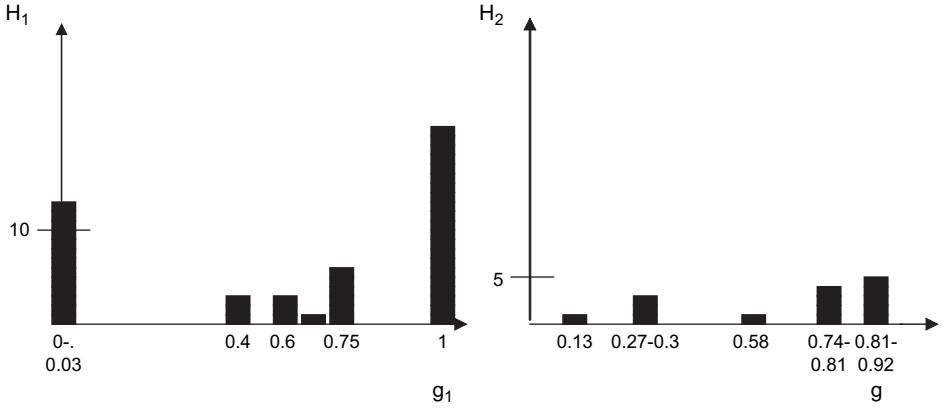


Fig. 9. $g_1$-spectrum [PV, BD] and $g_2$-spectrum [LC50, log Kow]. Ordinate axes are $H_1$ (left side) and $H_2$ (right side). Abscissa are $g_1$ and $g_2$.

Table 7
g1c and g2c − cluster

| Pairs due to g1c-values | Intervals g1c | Pairs due to g2c-values | Intervals g2c |
|---|---|---|---|
| 7 | 0.68…0.75 | 4 | 0.74…0.81 |
| 6 | 0.47…0.60 | 4 | 0.89…0.92 |
| 22 | 1 | 1 | 0.58 |
| 13 | 0 | 4 | 0.27…0.30 |
| | | 1 | 0.13 |

If $p = 2$ or greater, then one has to discuss $p$ different weights in $p$ 1-dimensional $g$-spaces. For example if $p = 2$ a graphic as shown in Fig. 8 may result. For example, exemplifying the procedure we start with two incomparabilities, namely 4NP||LIN and THI||MAL in the original Hasse diagram (Fig. 7).

Regarding 4NP||LIN we may calculate at least one crucial weight, according to (3). If we aggregate as follows: PV and BD on the one side ($\varphi_1$) and LC50 and log Kow on the other side ($\varphi_2$) then we see that with respect to PV and BD there is no incomparability: LIN $<_{PV,BD}$ 4NP. Then, the incomparability is due to antagonistic attributes (Simon et al., 2004) LC50 and log Kow. For that reason we calculate the crucial weight of LC50 and log Kow for LIN and 4NP. We find g2c = 0.745. For THI and MAL we find: THI$||_{PV,BD}$MAL but THI $<_{LC50,log\ Kow}$MAL. Therefore we associate with the pair (THI, MAL) the crucial weight g1c (separating the $g_1$-space) and its value turns out to be g1c = 0.75. A graphical representation for the pairs (LIN, 4NP) and (THI, MAL) is shown in Fig. 8.

Within the $G$-space [0,1] × [0,1] there are four fields, which arise from the separating lines due to g1c = const and g2c = const'. Within these four stability fields (see Section 4 below), the variation of the weights will not affect the order relations between THI-MAL on the one side and LIN-4NP on the other side. Hence we are speaking of a ''structure'' in the $G$-space. If $p > 2$ then a similar consideration leads to the generalization of stability (hyper-) cubes. Crossing a boundary (i.e. a line in $p = 2$, or a hyper-plane in $p > 2$) changes the relation for those pairs which belong to the corresponding crucial weight (see (6) in Section 2.4). If the variation of the weights crosses more than one crucial (hyper)plane of gkc-values then correspondingly many pairs of chemicals are affected in their order relations. Therefore crossing of (hyper-) planes are of special interest and are called ''hot spots'' in the ''$g$-space'' as explained in Section 2.5.

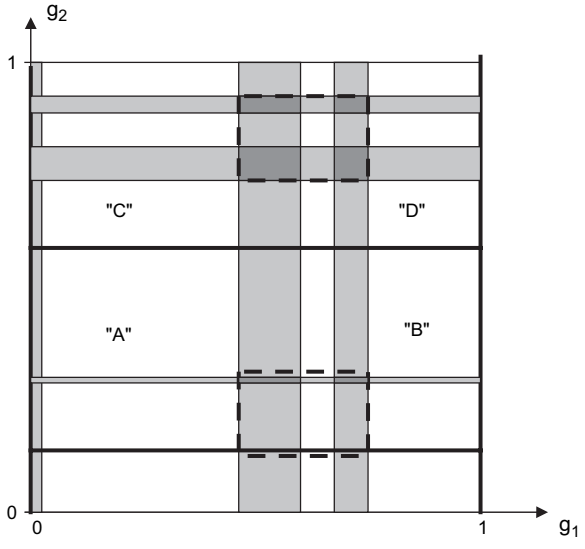


Fig. 10. Transition zones and stability fields for twelve chemicals. A, B, C, D are identifiers of stability fields (see Section 3.3).

### 3.3. g-spectra, stability fields and hot spots for twelve chemicals

We calculate the two $g$-spectra and represent them as histograms (see Fig. 9).

By a cluster analysis (complete linkage, squared Euclidian distance) a series of partitionings can be obtained. The cut level is selected so that an aggregation of non-trivial clusters is avoided. The partitioning in case of g1c contained 7, 6, 22, 13 object pairs, in case of g2c 4, 4, 1, 4, 1 object pairs. From any cluster the interval of its crucial $g$-values is determined. Hence the stability- and transition fields are found as follows (Table 7).

The diagrammatic representation of the results of the cluster analysis (Table 7 and Fig. 9) is shown in Fig. 10: the fields between the stripes are the stability fields.

Fig. 10 shows us that there are 18 stability fields (blank rectangular areas in Fig. 10) which can be characterized by just one Hasse diagram and there are 4 hot spots (dark rectangles in Fig. 10) which may also be merged to bigger hot spots (dashed lines). It should be clear that each transition zone contains a series of small stability fields, which are neglected in the course of the generalization. Variation of weights (by keeping the scheme of pairwise aggregation) will not change the relative positions of incomparable chemicals within a stability field (if the $g$-spectra allow defining such fields). If however the variation of weights crosses transition zones (the series of crucial gkc-values, grouped to stripes) the order relation of many pairs changes. A perhaps useful picture is that of a phase transition: varying the weights within a stability field the configuration will be invariant, crossing hot spots will change the configuration.

### 3.4. Typical Hasse diagrams

o-METEOR tends to reduce the problematic work of finding all weights simultaneously by a step-by-step procedure. Taking the data from the publication of Lerche et al. (2002a) the Hasse diagram shown in Fig. 7 and all subsequent Hasse diagrams are obtained. Here we show how after the introduction of the first two weights a set of possible posets will be obtained, so that only 18 typical Hasse diagrams are to be considered.

There are many incomparabilities which hamper a unique decision, albeit one may begin with the maximal elements {MAL, THI, CNB, DIA}. It is not meaningful to show every

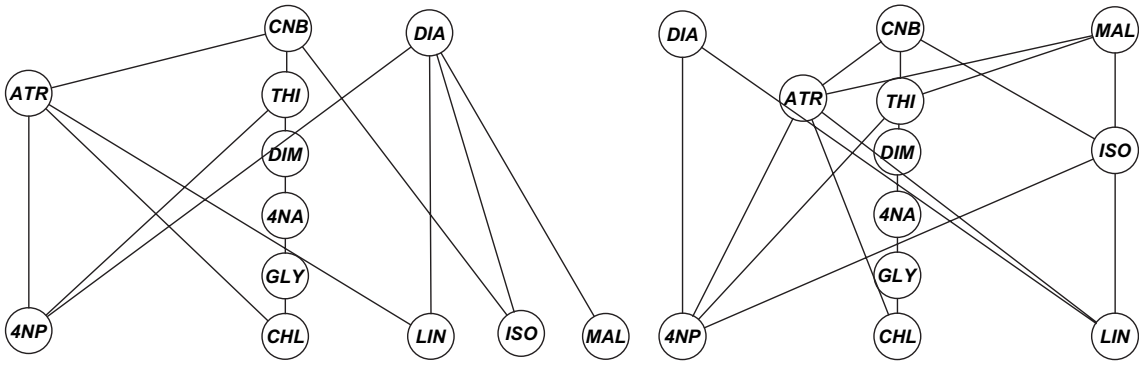


Fig. 11. Hasse diagram in stability field A (left), stability field B (right).

Hasse diagram. We only show the four most important ones; the importance we derive – as shown above – from the volumes of the (hyper-) cubes.

In stability field A ($0.03 < g1c < 0.47$) ($0.30 < g2c < 0.58$) the Hasse diagram is shown in Fig. 11 (left side), in stability field B in Fig. 11 (right side).

It is interesting to note that all three former hierarchies are now related to each other and in case of stability field A: that Malathion (MAL), which is isolated in (C, IB) is now comparable with Diazinon (DIA). This Hasse diagram results with a low weight for PV and a medium weight for LC50.

In the case of stability field B, where PV is considered as very important and BD as less important, Malathion (MAL) becomes a maximal element in the poset and is worse than many other chemicals. Comparing the Hasse diagram of field A with that of field B one observes many changes. This is consistent with the fact that between both stability fields a rather big transition zone is located, which implies that there are many pairs of incomparable elements, changing their order relations within the aggregation. Furthermore it should be noted that there are order preserving maps from the poset, shown in Fig. 7 to the posets shown in Fig. 11, but no order preserving map between the two Hasse diagrams of the stability fields A and B. This is consistent with the finding, summarized in Table 7 and schematically drawn in Fig. 12. In Fig. 13 the Hasse diagrams corresponding to the fields C and D (Fig. 10) are shown.

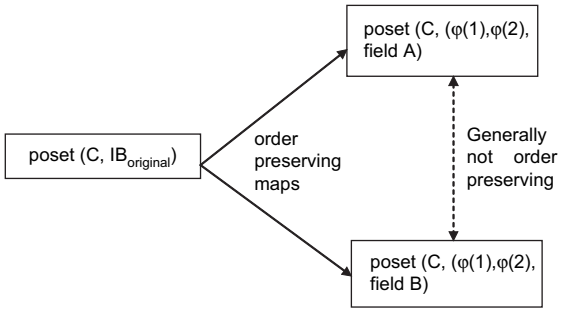


Fig. 12. Relation between original poset and posets after aggregation using different weights.

Once again, passing the large transition zone (from A/C to B/D) implies many changes, however the boundary which separates A from C and B from D is just one chemical pair. Hence it is clear that the vertical transition will only exhibit one change. Namely LIN||THI is converted to THI > LIN and vice versa. It is interesting to note how an aggregation affects the position of the chemical MAL. In the original Hasse diagram (Fig. 7) it is an isolated element, hence any aggregation may change the position of MAL drastically (compare Brüggemann et al., 2001). In stability field C the chemical MAL is a minimal element, whereas in stability field D it is a maximal one. This finding also shows, how crucial a weighting can be and how important it is, to analyze object sets by partial order set theory!

## 4. Discussion and conclusion

In contrast to its kernel, the HDT, METEOR allows participation of stakeholders and provides the stepwise introduction of weights. The expectation is that often just some few steps will be helpful for the decision (here: which chemical is hazardous to the environment). For example incomparable chemicals as shown in Fig. 7 are now related to each other in a systematic, i.e. order preserving way. The example shows an intermediate state of o-METEOR, namely after introduction of only two weights, whereas for a linear ranking three weights would be needed (weights are normalized so that their sum equals 1). The advantages associated with discrete approaches such as the HDT, which provide high transparency throughout the whole evaluation process is combined with the flexible use of weights, which model the subjective preferences.

From the more mathematical/statistical and software technical point of view there are many questions open, which are to be solved in the future:

1) What is the most efficient strategy for aggregation? Will the bottom-up strategy always be rather inefficient, whereas the top-down strategy resolves in its first steps the most important conflicts? Here it may be useful to discuss the aggregation procedure in terms of conflict diagrams as introduced by Sørensen et al. (2005).

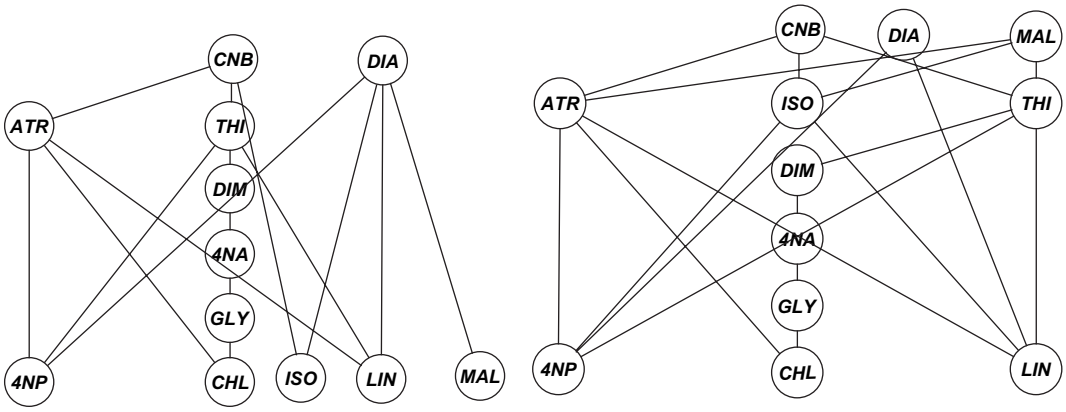


Fig. 13. Left side: Hasse diagrams of stability field C; Right side: stability field D.

2) As discussed in Section 2.4 the Eq. (2) alone leads only to a lower bound of possible order theoretical extensions. In order to obtain all extensions (not necessarily only the linear ones) each configuration must be expressed by a bundle of inequalities describing the order relations. This however, on the one side in large posets is a computational problem and on the other side not all linear extensions will be obtained by just a linear combination of the attributes. Therefore we think and suggest that equations of type (2) (Section 2.4) are a good compromise.
3) Which relations can be found among the posets obtained in intermediate steps of aggregation? Certainly there must be a set of order preserving maps between the original poset and the derived posets due to different aggregations. However the degree of enrichment of comparabilities will be different, as could be seen in Fig. 7 in comparison to the posets shown in Figs. 11 and 13. Hence it is of interest to characterize aggregation schemes at least in terms of similarity within the set of crucial weights.
4) How far the concept of stability fields (or ''phases'') and phase transitions can be further applied? We have seen that the broadness of transition zones corresponds to the number of changes by which the poset will be affected. Hence the stripes and their geometrical configurations are of main interest.
5) If we do not know any weight. Which stability field should be examined first? The volume (or in technical terms: measure) of the stability hypercubes (here planes) may give a useful advice. Here the largest stability field is field A: $(0.47 - 0.03) * (0.58 - 0.30 = 0.132)$ followed by field B: $(1 - 0.75) * (0.58 - 0.30) = 0.07$. Therefore we started in Section 3.3 with the largest stability field ''A'' by determining the Hasse diagrams and continue with three stability fields of lower measures.
6) What's about the generalization to $p > 2$. In this paper we exemplified the ideas by $p = 2$, many graphical schemes are based on a two-dimensional representation. In real life $p$ will be by far greater than 2. If the o-METEOR approach is followed then $p$ one-dimensional g-spaces are to be calculated and characterized by their gkc-values. If more general aggregations (including two- or higher dimensional $g$-spaces) are to be used, then the transition zones have to be calculated and it is more difficult to present them graphically.
7) Can we always expect stability fields? Yes and no! Clearly we get with a finite set of objects (i.e. of chemicals) only discrete sets of crucial weights. Hence one may find within two adjacent crucial weights always a more or less large field of invariant $<$ or $>$-relations. However, if the crucial weights in all dimensions are approximately homogenously filling out the interval [0,1] in any $g$-space then any small change of weights everywhere in the $G$-space will lead to a phase transition. In that case one may perform a classification of the original attributes into scores or define an aggregation which does not pairwise combine the original attributes. This however, leads to a theoretically more complex system, which is still open for further research.
8) METEOR may be seen as one example of the $g$-posets. We speak of $g$-posets, if the attributes by which a componentwise order is defined, are dependent on a set of continuous varying parameters. If for example a poset and its visualization by Hasse diagrams is used to exhibit structure-fate relations of chemicals in the environment (Brüggemann et al., 2006a) then a natural question arises how the poset depends on environmental parameters, if the characterizing attributes are fate descriptors. In METEOR and especially in o-METEOR the relations can be considered as relatively simple because of the linearity of the $\varphi$-functions with respect to the weights. In the case of structure–fate relationships the descriptors in general will non-linearly depend on parameters like water discharge, organic carbon content etc. First attempts are under development (Restrepo et al., 2007b). However the field of $g$-posets needs the joint work of many scientists in the future. We hope that in the series of workshops about partially ordered sets in chemistry and environmental sciences (initialized by the first author) this joint cooperation can be enhanced.
9) o-METEOR is intended to serve as a decision support tool for environmental sciences too. However, before

we recommend its application as a decision support tool we have to compare it with several other well-known procedures, e.g. PROMETHEE. That means we have to continue the work begun by Lerche et al. (2002a) where HDT was compared with four other decision support tools.

## Acknowledgments

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## Appendices

## Appendix 1

a. Abbreviations (alphabetically sorted)

| Abbreviation | Explanation |
|---|---|
| AHP | Analytic hierarchy process |
| Bottom-up-procedure | Starting from very detailed information and aggregate those attributes, which belong to the same subcriterion |
| ELECTRE | (French): Elimination et Choix Traduisant la Realité |
| Extremal case procedure | The aggregation procedure in METEOR will be stopped if a) a greatest or least element is found or b) if two elements of interest can be compared. |
| HD | Hasse diagram |
| HDT | Hasse diagram technique |
| HPVC | High production volume chemicals |
| MAUT | Multiattribute utility function theory |
| MCDA | Multi-criteria decision aids |
| METEOR | Method of evaluation by order theory |
| NAIADE | Novel approach to imprecise assessment and decision environment |
| o-METEOR | Like METEOR, however a specific aggregation scheme |
| poset(s) | Partially ordered set(s) |
| PROMETHEE | Preference ranking organisation method for enrichment evaluation |
| REACH | Registration, evaluation, authorisation of chemicals |
| Top-down-procedure | Aggregate that pair of attributes which is most anticorrelated, then the next pair of attributes, etc. |
| WHASSE | Hasse for Windows |

b. Symbols and concepts

| Symbol | Explanation | Remarks |
|---|---|---|
| $g_k^c$ | Crucial weight | Eq. (4) (often simply written gkc) |
| $\Delta_i^{x,y}$ | $=q_i(x) - q_i(y)$ | |
| $Q_{ij}^{x,y}$ | $= \Delta_i^{x,y} / \Delta_j^{x,y}$ | |
| $\varphi_k$ | Weighted sum of $q_i \in k$ | |
| $\|\|$ | Sign to denote incomparability | |
| BD | Biodegradation | |
| C | Set of objects | In Section 3: set of Chemicals |
| $g_i$ | The weights | They are representing in this study the external knowledge |
| $g$-space | $g \in [0,1]^p \subset IR^p$ | $IR^p$ set of $p$-tuples of real numbers. In o-METEOR the $g$-spaces are one-dimensional |
| $G$-space | Product of all $g$-spaces | $\subset IR^m$ |
| $H_k(g(k))$ | Number of pairs of ICk, having the same gkc-value | $g$-spectrum: $H_k$ versus $g_i \in [0,1]$ |
| Hot spots | Subspaces of the $G$-space where a change of weights changes the relative positions of two incomparable objects | |
| IB | Set of attributes, characterizing objects in order to perform an evaluation | |
| $IC_k$ | Set of pairs of incomparable objects, due to set $k$ | Equation 6 |
| LC50 | The dose of a substance which is fatal to 50% of the test animals | |
| log Kow | log of $n$-octanol/water partitioning coefficient | |
| $m$ | Number of attributes | $m =$ card IB |
| $N$ | Number of objects | $N =$ card C |
| $p$ | Dimension of the $G$-space | |
| PV | production volume | |
| $q_i$ | $i$th attribute | The attributes $q_i$ represent in our study the primary knowledge |
| $q_i(x)$ | The value of the $i$th attribute for object x | |
| $q_i$(max) | The maximum value of $q_i$ within a set of objects | |
| $q_i$(min) | The minimum value of $q_i$ within a set of objects | |

**Appendix 1** (*continued*)

| Symbol | Explanation | Remarks |
|---|---|---|
| $S_k$ | A set of those attributes which are to be combined by a weighted sum | |
| Stability fields | Subspaces of the *G*-space where a change of weights does not change the relative positions of two incomparable objects | |
| Stripes | If gkc-values are close to each other one may define an interval and represent all these values by just one area in the *G*-space, where-crossing this area by variation of weights-many changes in the order relations appear | Also called a transition zone |

## Appendix 2

Given the set IB of $m$ attributes the total number of possible subsets of it is given by the cardinality of the power set of IB (P(IB)), which corresponds to $2^m$. We write $2^m$-$m$-2 since we do not consider the original attributes in IB either the empty set either the subset containing all the attributes as simultaneously aggregated. If we suppose IB $= \{q_1, q_2, q_3\}$ then the possible number of subsets of those three attributes is $2^3 = 8$, which are P(IB) $= \{\{q_1\}, \{q_2\}, \{q_3\}, \{q_1, q_2\}, \{q_1, q_3\}, \{q_2, q_3\}, \{q_1, q_2, q_3\}, \varnothing\}$. From P(IB) just $\{q_1, q_2\}$, $\{q_1, q_3\}$, and $\{q_2, q_3\}$ can be considered as aggregation of the attributes $q_1$, $q_2$ and $q_3$. Hence, their number is $2^3$-3-2 $= 3$. Note, however that these three possible aggregations are not disjoint.

## Appendix 3

Given the set IB of $m$ attributes, a partition D of IB is a collection of subsets of IB such that:

$$\text{(i)} \quad \text{If } S_1, \ldots, S_m \subset \text{IB}, \qquad \text{then } \bigcap_{k=1}^{m} S_k = \varnothing$$

$$\text{(ii)} \quad \text{If } S_1, \ldots, S_m \subset \text{IB}, \qquad \text{then } \bigcup_{k=1}^{m} S_k = \text{IB}$$

Thus, if we IB $= \{q_1, q_2, q_3\}$ we have the following partitions: D1 $= \{q_1, q_2, q_3\}$, D2 $= \{\{q_1\}, \{q_2, q_3\}\}$, D3 $= \{\{q_2\}, \{q_1, q_3\}\}$, D4 $= \{\{q_3\}, \{q_1, q_2\}\}$ and D5 $= \{\{q_1\}, \{q_2\}, \{q_3\}\}$.

## Appendix 4

The number of ways a set IB of m attributes can be partitioned into $k$ non-empty sets is $S_2(m, k)$, which is called a Stirling number of the second kind.

$$S_2(m,k) = (1/k!) \sum_{i=0}^{k} (-1)^i \binom{k}{i} (k-i)^m.$$

If IB $= \{q_1, q_2, q_3\}$ and we decide to aggregate its elements in two classes, then $S(3,2) = 3$ and the partitions are D2, D3 and D4 form A2.

## Appendix 5

The number of ways a set IB of $m$ attributes can be partitioned into non-empty subsets is called a Bell's number ($B(m)$). $B(m) = \sum_{k=1}^{m} S_2(m,k)$, being $S_2(m, k)$ defined in A4. If IB $= \{q_1, q_2, q_3\}$, then $B(3) = 5$ and the partitions appear in A2.

## References


Berlekamp, J., Lautenbach, S., Graf, N., Reimer, S., Matthies, M., 2007. Integration of MONERIS and GREAT-ER in the decision support. Environ. Model. Software 22, 239–247.

Bock, H.H., 1974. Automatische Klassifikation. Vandenhoeck&Ruprecht, Göttingen, pp. 6–480.

Brans, J.P., Vincke, P.H., 1985. A preference ranking organisation method (The PROMETHEE method for multiple criteria decision-making). Manag. Sci. 31, 647–656.

Brüggemann, R., Carlsen, L., 2006. Partial Order in Environmental Sciences and Chemistry. Springer-Verlag, Berlin, pp. 1–406.

Brüggemann, R., Drescher-Kaden, U., 2003. Einführung in die modellgestützte Bewertung von Umweltchemikalien – Datenabschätzung, Ausbreitung, Verhalten, Wirkung und Bewertung. Springer-Verlag, Berlin, pp. 1–519.

Brüggemann, R., Voigt, K., 1995. An evaluation of online databases by methods of lattice theory. Chemosphere 31 (7), 3585–3594.

Brüggemann, R., Welzl, G., 2002. Order theory meets statistics-Hasse diagram technique. In: Voigt, K., Welzl, G. (Eds.), Order Theoretical Tools in Environmental Sciences – Order Theory (Hasse Diagram Technique) Meets Multivariate Statistics. Shaker-Verlag, Aachen, pp. 9–39.

Brüggemann, R., Münzer, B., Halfon, E., 1994. An algebraic/graphical tool to compare ecosystems with respect to their pollution – the German River 'Elbe' as an example – I: Hasse-Diagrams. Chemosphere 28, 863–872.

Brüggemann, R., Bücherl, C., Pudenz, S., Steinberg, C., 1999. Application of the concept of partial order on comparative evaluation of environmental chemicals. Acta Hydrochim. Hydrobiol. 27, 170–178.

Brüggemann, R., Halfon, E., Welzl, G., Voigt, K., Steinberg, C., 2001. Applying the concept of partially ordered sets on the ranking of near-shore sediments by a battery of tests. J. Chem. Inf. Comp. Sci. 41, 918–925.

Brüggemann, R., Sørensen, P.B., Lerche, D., Carlsen, L., 2004. Estimation of averaged ranks by a local partial order model. J. Chem. Inf. Comp. Sci. 44, 618–625.

Brüggemann, R., Simon, U., Mey, S., 2005. Estimation of averaged ranks by extended local partial order models. Match – Comm. Math. Co. 54, 489–518.

Brüggemann, R., Restrepo, G., Voigt, K., 2006a. Structure-fate relationships of organic chemicals derived from the software package E4CHEM and WHASSE. J. Chem. Inf. Model 46 (2), 894–902.

Brüggemann, R., Simon, U., Nützmann, G., 2006b. Analyzing water management strategies in urban regions by directed graphs. In: Studzinski, J., Hryniewicz, O. (Eds.), Modelling Concepts and Decision Support in

Environmental Systems, vol. 45. Polish Academy of Science, Warsaw, pp. 111–124.

Castelletti, A., Soncini-Sessa, R., 2006. A procedural approach to strengthening integration and participation in water resource planning. Environ. Model. Software 21, 1455–1470.

De Loof, K., de Meyer, H., de Baets, B., 2006. Exploiting the lattice of ideals representation of a poset. Fundam. Inform. 71, 309–321.

EEC, 2001. WHITE PAPER, Strategy for a Future Chemicals Policy, Brussels, 27.2.2001, COM(2001) 88 final. http://www.reachcentrum.eu/media/whitepaper.pdf.

European Commission, 2006. REACH in brief, September 2006, http://ecb.jrc.it/DOCUMENTS/REACH/REACH_in_brief_council_comm_pos_060905.pdf.

Giupponi, C., 2007. Decision Support Systems for implementing the European Water Framework Directive: The MULINO approach. Environ. Model. Software 22, 248–258.

Klauer, B., Messner, F., Drechsler, M., Horsch, H., 2001. Das Konzept des integrierten Bewertungsverfahrens. In: Horsch, H., Herzog, F. (Eds.), Nachhaltige Wasserbewirtschaftung und Landnutzung. Methoden und Instrumente der Entscheidungsfindung und Umsetzung. Metropolis, Marburg, pp. 75–99.

Lerche, D., Brüggemann, R., Sørensen, P.B., Carlsen, L., Nielsen, O.J., 2002a. A comparison of partial order technique with three methods of multicriteria analysis for ranking of chemical substances. J. Chem. Inf. Comp. Sci. 42, 1086–1098.

Lerche, D., Sørensen, P.B., Larsen, H.L., Carlsen, L., Nielsen, O.J., 2002b. Comparison of the combined monitoring – based and modelling – based priority setting scheme with partial order theory and random linear extensions for ranking of chemical substances. Chemosphere 49, 637–649.

Lerche, D., Sørensen, P.B., Brüggemann, R., 2003. Improved estimation of the ranking probabilities in partial orders using random linear extensions by approximation of the mutual probability. J. Chem. Inf. Comp. Sci. 53, 1471–1480.

Makropoulos, C.K., Butler, D., 2006. Spatial ordered weighted averaging: incorporating spatially variable attitude towards risk in spatial multi-criteria decision-making. Environ. Model. Software 21, 69–84.

Matarazzo, B., Munda, G., 2001. New approaches for the comparison of L-R fuzzy numbers: a theoretical and operational analysis. Fuzzy Sets Syst. 118, 407–418.

Ocampo-Duque, W., Schuhmacher, M., Domingo, J.L., 2007. A neural-fuzzy approach to classify the ecological status in surface waters. Environ. Pollut. 148, 634–641.

Reichert, P., Borsuk, M., Hostmann, M., Schweizer, S., Spoerri, C., Tockner, K., Truffer, B., 2007. Concepts of decision support for river rehabilitation. Environ. Model. Software 22, 188–201.

Restrepo, G., Brüggemann, R., Weckert, M., Gerstmann, S., Frank, H., 2007a. Refrigerants ranked by partial order theory. In: Hryniewicz, O., Studzinski, J., Szediw, A. (Eds.), EnviroInfo 2007. Environmental Informatics and Systems Research, vol. 2. Shaker-Verlag, Aachen, pp. 209–217.

Restrepo, G., Brüggemann, R., Voigt, K., 2007b. Partially ordered sets in the analysis of alkanes' fate in rivers. Croatia Chem. Acta 80 (2), 261–270.

Roy, B., 1990. The outranking approach and the foundations of the ELECTRE methods. In: Bana e Costa, C.A. (Ed.), Readings in Multiple Criteria Decision Aid. Springer, Berlin, pp. 155–183.

Saaty, T.L., 1994. How to make a decision: the analytical hierarchy process. Interfaces 24, 19–43.

Schneeweiss, C., 1991. Planung 1 – Systemanalytische und entscheidungstheoretische Grundlagen. Springer, Berlin.

Simon, U., Brüggemann, R., Pudenz, S., 2004. Aspects of decision support in water management – example Berlin and Potsdam (Germany) I – spatially differentiated evaluation. Water Res. 38, 1809–1816.

Simon, U., Brüggemann, R., Mey, S., Pudenz, S., 2005. METEOR – application of a decision support tool based on discrete mathematics. Match – Comm. Math. Co. 54, 623–642.

Sørensen, P.B., Brüggemann, R., Thomsen, M., Lerche, D., 2005. Applications of multidimensional rank-correlation. Match – Comm. Math. Co. 54, 643–670.

Vink, J.P.M., Meeussen, J.C.L., 2007. BIOCHEM-ORCHESTRA: a tool for evaluating chemical speciation and ecotoxicological impacts of heavy metals on river flood plain systems. Environ. Pollut. 148, 833–841.

Voigt, K., Brüggemann, R., 2005. Water contamination with pharmaceuticals: data availability and evaluation approach with Hasse diagram technique and METEOR. Match – Comm. Math. Co. 54, 671–689.

Voigt, K., Brüggemann, R., Pudenz, S., 2004a. Chemical databases evaluated by order theoretical tools. Anal. Bioanal. Chem. 380, 467–474.

Voigt, K., Welzl, G., Brüggemann, R., 2004b. Data analysis of environmental air pollutant monitoring systems in Europe. Environmetrics 15, 577–596.

Voigt, K., Brüggemann, R., Pudenz, S., 2006. A multi-criteria evaluation of environmental databases using the Hasse diagram technique (ProRank) software. Environ. Model. Software 21, 1587–1597.

Znidarsic, M., Bohanec, V., Zupan, B., 2006. ProDEX – A DSS tool for environmental decision-making. Environ. Model. Software 21, 1514–1516.