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Research article

A posetic based assessment of atmospheric VOCs

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Abstract: The assessment of a series of volatile organic compounds (VOCs) based on partial order methodology is reported using available data from six sites in Yokohama, Japan as an exemplary case. The individual VOCs are mutually ranked according to their importance, the ranking being made both based on the recorded concentration and the concentrations adjusted for the possibility of the single VOCs to exhibit respiratory toxicity. The relative importance of the single sites is disclosed to verify the overall most problematic area from an air pollution point of view. The concentration profiles for the six sites are scrutinized for possible 'peculiar' profiles. As air pollution data typically are associated with significant uncertainty the possible effects of data noise/uncertainty is addressed.

Keywords: air pollution; VOC; partial ordering; ranking; peculiar VOCs; data uncertainty

1. Introduction

Air pollution appears as one of the major health hazards. Thus, it has been estimated by the World Health Organization (WHO) that air pollution in 2012 caused the death of 3.7 million people under the age of 60 [1]. It has been reported that volatile organic compounds, VOCs, constitute one of the most hazardous groups of air pollutants [2-5]. The health effects of VOCs are obvious connected to the actual concentrations of the single compounds. However, also the toxicity may play a role. Further it is noted that VOCs plays an important role in smog formation [6].

Often the effects like toxicity are studied for single compounds. However, urban VOCs constitute a mixture of a wide variety of compounds, where the disclosure of the relative importance of the single compounds may be missing. However, in order to combat the VOC pollution such knowledge obviously is crucial in planning where to focus the effort to get the highest effects in terms of reducing the overall toxicity due to VOCs.

The present paper describes the assessment of atmospheric VOCs based on 6 sites in Yokohama, Japan as an exemplary case [7] applying partial order methodology. The major advantage of applying partial order methodology for such studies is that no additional assumptions are made. Thus, the only input to the analyses is the actual data. Especially possible compensation effects due to indicator aggregation are avoided (vide infra). The assessment is based on concentrations as well as the concentration adjusted for the probability of possessing respiratory toxicity and elucidates also the relative importance of the six sites as well as a discussion on the possible presence of "peculiar" compounds present in certain areas. The possible influence of data noise/uncertainty is addressed.

2. Methods

The study includes six specific sites in Yokohama, Japan [7]. The sites 1, 2 and 3 are located on the coast of the Yokohama city characterized by the presence of especially petrochemical industrial activity. The sites 4 and 6 are both located in residential areas, site 4 with low traffic flow but influenced by the surrounding area and site 6 close to the industrial site 3. Site 5 is a commercial site with significant traffic load (for details [7] should be consulted). As we are having a system comprising six indicators (the six sites) and 34 elements (the VOCs) we are dealing with a multi-indicator system, a MIS.

2.1. Data

The actual data [7] are associated with a significant uncertainty, i.e., up to 100%. However, as starting point the present study applies the given concentration. The effects of the data uncertainty will be dealt with separately. The actual uncertainty ranges up to 100% [7]. In Table 1 the applied MIS is given together with the probability for the single VOCs to exhibit respiratory toxicity. It should be noted that C2-VOCs included in the original study has been excluded here as the applied QSAR model (vide infra) does not allow reliable calculation for compounds with less than 3 carbons [8]. In Table 2 the original ID labelling corresponding to that in [7] is maintained after eliminating the C2-VOCs.

The probabilities for the single VOCs to exhibit respiratory toxicity was generated through quantitative structure-activity relationships (QSAR) applying the freely available version of PASS software [8] calculation adverse effects and toxicities.

2.2. Partial order methodology

2.2.1. Motivation

Comparisons of elements characterized by several parameters/indicators (multi-indicator systems) are often done based on a simple numerical aggregation leading to one single indicator as a weighted sum. However, this may lead to unwanted compensation effects [9]. Further it may be a difficult process to find appropriate weights. Thus alternative methodologies obviously should be looked for. Partial ordering methodology could be such an alternative. The methodology does not require pre-processing nor aggregation of data. In the following the data presented in Table 1 are analysed.

Table 1. Concentration (ppb) of VOCs at six sites in Yokohama Japan [7]. The last column gives the probability for exhibiting respiratory toxicity evaluated by PASS [8].

VOC	ID	Site 1	Site 2	Site 3	Site 4	Site 6	Site 5	respTox
Propane	2	5.5	2.1	24.7	1.9	5	2.8	0.901
Isobutane	3	2.1	1.8	4.6	0.9	1	1.9	0.859
n-Butane	4	5.3	3.5	6	1.5	1.6	3.8	0.922
Isopentane	5	7.2	3.4	3.7	1.4	1.4	4.2	0.874
n-Pentane	6	3.2	1.8	2.6	0.6	0.8	1.5	0.932
2-Methyl pentane	7	1.4	1.8	1.2	0.4	0.5	0.9	0.912
3-Methyl pentane	8	0.7	0.6	0.5	0.3	0.3	0.4	0.948
n-Hexane	9	1.7	1.1	2.4	0.7	1.2	1.2	0.932
Methylcyclopentane	10	0.4	0.3	1.3	0.2	0.2	0.3	0.642
n-Heptane	11	0.3	0.2	0.4	0.2	0.2	0.2	0.932
n-Octane	12	0.3	0.1	0.2	0.1	0.1	0.1	0.932
n-Nonane	13	0.4	0.2	0.2	0.1	0.1	0.2	0.932
n-Decane	14	0.4	0.2	0.2	0.1	0.2	0.2	0.932
n-Undecane	15	0.2	0.1	0.2	0.1	0.2	0.2	0.932
n-Dodecane	16	0.1	0.1	0.2	0.1	0.1	0.1	0.932
n-Tridecane	17	0.2	0.1	0.2	0.1	0.1	0.1	0.932
n-Tetradecane	18	0.2	0.2	0.2	0.1	0.2	0.2	0.932
Propylene	21	0.8	2.2	2	2.4	1	1.2	0.766
1.Isobutene	22	0.4	0.4	2	0.2	0.4	0.4	0.886
Benzene	23	0.7	0.4	2.1	0.4	0.9	0.7	0.848
Toluene	24	3.1	1.6	5.2	1.9	2.2	2.2	0.92
Ethyl benzene	25	0.8	0.7	2.9	0.5	0.9	0.5	0.939
m.p-Xylene	26	0.8	0.5	2.1	0.4	0.7	0.6	0.918
o-Xylene	27	0.4	0.3	0.7	0.2	0.3	0.3	0.828
m-Ethyl toluene	28	0.3	0.2	0.2	0.1	0.1	0.2	0.952
p-Ethyl toluene	29	0.3	0.2	0.2	0.2	0.2	0.2	0.948
o-Ethyl toluene	30	0.2	0.1	0.1	0.1	0.1	0.1	0.864
1.3.5-Trimethyl benzene	31	0.1	0.1	0.1	0.1	0.1	0.1	0.912
1.2.4-Trimethyl benzene	32	0.5	0.3	0.3	0.2	0.2	0.3	0.846
Naphthalene	33	0.2	0.2	0.2	0.2	0.2	0.2	0.892
Ethylacetate	34	0.4	0.6	0.6	0.6	0.6	0.6	0.967
Methylethylketone	35	1.1	0.6	1.4	0.8	1	0.8	0.606
n-Nonylaldehyde	36	0.1	0.1	0.1	0.1	0.1	0.1	0.818
p-Dichlorobenzene	39	0.1	0.1	0.1	0.15	0.1	0.1	0.849

2.2.2. Technicalities

The basis for partial ordering is the relation among the objects to be ordered. We call the set of objects X. The only mathematical term in this context is "≤" [10-14]. Thus, the "≤"-relation is the basis for a comparison of objects and constitutes a graph, the so-called Hasse diagram (see below). Two objects are connected with each other if and only if the relation $x \leq y$ holds. However, since

each object is characterized by a series of indicators r_j, the obvious question is how $x \leq y$ should be understood. As a given object, x, is characterized by a set of indicators $r_j(x)$, j = 1,...,m, it can be compared to another object, y, characterized by an identical set of indicators $r_j(y)$, if

$$r_i(x) \leq r_i(y) \text{ for all } i = 1,\ldots,m \quad (1)$$

Equation 1 is the basis for the so-called Hasse diagram technique (HDT) [10-14]. By identifying the set of indicator values with the objects, it can also be written $x < y$, when equation 1 is fulfilled. HDT is a special (statistically oriented part of partial order theory). Hasse diagrams are visual representation of the partial order, where comparable objects are connected by a sequence of lines [11,12,14-16]. Consequently, incomparable objects appear non-connected in the Hasse diagram. For construction of a sensible Hasse diagram, it is mandatory that all indicators have a uniform orientation, i.e., high indicator values correspond, e.g., to "bad" (e.g., high concentrations) elements, and low values - to "good" (e.g., low concentrations) elements (or vice versa). In the present study, high VOC concentrations are regarded as bad whereas low concentrations as good.

Typically, the structure of a Hasse diagram allows—beside others—the identification of

- maximal elements, no other elements are comparable and located above them,
- minimal elements, no other elements are comparable and located below them and
- isolated elements, which are minimal and maximal elements simultaneously.
- levels, which are the horizontal arrangement of objects within the diagram (for details, see [11])
- chains, which are special subsets of the partially ordered set (poset), where all objects in the subset fulfill Equation 1. Chains can be characterized by the length, i.e., by the number of members of the chains.
- antichains are subsets of X, where no object fulfills Equation 1.

The level structure gives a first approximation to a weak order of the objects from "good" (bottom) to "bad" (top). However, this construction will obviously lead to many tied orders tied orders (therefore often called a "weak order") as all objects in a level automatically will be assigned an identical order [17]. If all indicator values are identical for two or more elements these will be denoted equivalent and only a representative will appear in the Hasse diagram.

Based on the data in Table 1, the Hasse diagram shown in Figure 1 is constructed. A detailed evaluation of the Hasse diagram (Figure 1) is given below.

2.3. Posetic tools to be applied

In the present study, some partial ordering methodologies are used that are all well described in recent publications. The posetic tools applied in in the present study are

- Construction and basic analyses of Hasse diagrams [10-14] applying module mHDCl5_4 of the PyHasse software package.
- Average heights [18] applying module LPOMext_without_psyco7_1 of the PyHasse software package. Based on the calculated average heights the ranks of the single compounds are calculated using the approach of average ranks for tied height-values in order to free the ranking from irrelevant numerical values [19,20]. It should be noted that the average heights are given from the bottom to the top, whereas the eventual ranking is reversed.

- Peculiar compounds [21] to elucidate possible unbalanced indicator profile of the studied cities applying module incompposet5_1 of the PyHasse software package.
- Sensitivity analysis [22] to elucidate the relative importance of the single sites (indicators) applying module sensitivity20_5 of the PyHasse software package.
- Effects of possible data uncertainties/noise [23,24] applying module MC_basedHD11_1 of the PyHasse software package.

For in depth descriptions of the various methodologies, the original references cited above should be addressed.

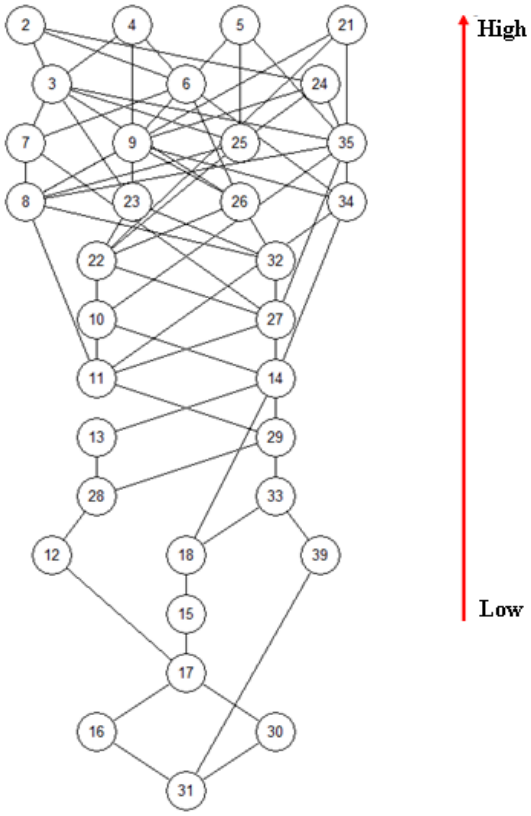

Figure 1. Hasse diagram based on the MIS (Table 1). The diagram has 442 comparabilities and 86 incomparabilities. Note: compound 31 and 36 are equivalent.

2.4. Software

In the present study a series of partial ordering tools has been applied, using selected modules of the PyHasse software package [25] programmed using the interpreter language Python (version 2.6) [26-30]. Today, the software package contains more than 100 specialized modules designed to solve specific tasks in the context of partial ordering. This 'pro' version is available upon request from the developer, Dr. R. Bruggemann (brg_home@web.de). A simplified version of PyHasse operating on a web-based browser is further under development. Some few tools are now available (see www.pyhasse.org). Both the 'pro' version and the web-based tool are under continuous development.

3. Results and Discussion

3.1. Analyses based on the original MIS

Looking at the Hasse diagram depicted in Figure 1 at is noted that the diagram is rather slim and pretty high with 14 levels. This is a result of a relative high correlation between the six indicators (Table 2). This may a priori be somewhat surprising as it could be expected that certain VOCs would be dominating the pattern originating from the industrialized areas (Site 1, 2 and 3). However, obviously this is not the case. Thus, the overall composition of the Yokohama VOC pollution is to a large extent independent of the actual area studied.

Table 2. Spearman correlation matrix (applied normalized MIS) for the six indicator sites.

	Site 1	Site 2	Site 3	Site 4	Site 6
Site 1	1.0	0.946	0.925	0.864	0.901
Site 2	0.946	1.0	0.916	0.923	0.927
Site 3	0.925	0.916	1.0	0.883	0.937
Site 4	0.864	0.923	0.883	1.0	0.936
Site 6	0.901	0.927	0.937	0.936	1.0
Site 5	0.955	0.976	0.943	0.923	0.961

It is in the connection interesting to look at the relative importance of the six indicator sites to elucidate how important the single sites are in the overall explanation of the VOC pollution as illustrated by the Hasse diagram in Figure 1.

The relative importance of the six sites is illustrated in Figure 2. It is thus disclosed that the importance is Site 1 > Site 3 > Site 4 > Site 6 > Site 2 > Site 5, the corresponding normalized values being 0.345, 0.276, 0,195, 0.092, 0.069, 0.023, respectively.

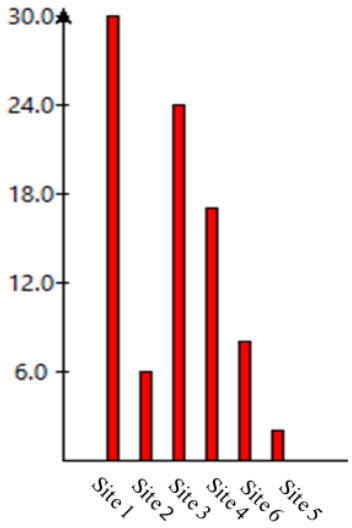

Figure 2. Relative importance of the six investigated sites taking only the VOC concentrations into account.

It is important to stress that these figures do not tell that, e.g., Site 1 is the more polluted. The figures simple elucidates the relative importance of the six sites in explaining the overall VOC pollution pattern in Yokohama as being studied based on these specific six sampling sites.

The next step is to disclose what VOCs are the most significant in Yokohama based on the measurements from the six sites. In Table 3 the average heights as well as the ranks of the 34 VOCs are given.

Table 3. Average heights and corresponding ranking of the 34 VOCs based on the original MIS (Table 1).

VOC	ID	Average height	Average height uncertainty	Rank
Propane	2	32.326	30...33	1
n-Butane	4	31.867	29...33	2
Isopentane	5	31.389	28...33	3
Toluene	24	29.817	26...32	4
Isobutane	3	29.017	26...31	5
Propylene	21	28.133	21...33	6
n-Pentane	6	27.262	23...30	7
n-Hexane	9	26.475	23...29	8
Methylethylketone	35	24.293	20...28	9
Ethyl benzene	25	24.183	20...28	10
Benzene	23	22.792	19...27	11
2-Methyl pentane	7	22.743	18...28	12
m.p-Xylene	26	22.228	19...26	13
1.Isobutene	22	19.076	17...22	14
Ethylacetate	34	18.283	15...24	15
3-Methyl pentane	8	18.276	16...22	16
Methylcyclopentane	10	16.467	15...20	17
o-Xylene	27	16.176	15...19	18
1.2.4-Trimethyl benzene	32	15.676	14...19	19
n-Heptane	11	13.824	12...15	20
n-Decane	14	12.867	10...14	21
p-Ethyl toluene	29	12.314	11...13	22
Naphthalene	33	10.571	8...12	23
n-Nonane	13	10.433	7...13	24
n-Tetradecane	18	8.048	6...10	25
m-Ethyl toluene	28	8.025	6...10	26
n-Undecane	15	6.238	5...9	27
n-Octane	12	6.2	5...9	28
p-Dichlorobenzene	39	5.567	2...11	29
n-Tridecane	17	4.3	4...5	30
n-Dodecane	16	2.611	2...4	31.5
o-Ethyl toluene	30	2.611	2...4	31.5
1.3.5-Trimethyl benzene	31	1	1...1	33.5
n-Nonylaldehyde	36	1	1...2	33.5

It can be noted (Table 3) that the more significant pollutants are the relatively light aliphatic hydrocarbons apart from toluene with rank 4. Benzene is found at rank 11. With reference to the toluene and benzene data (Table 1) this strongly indicates that, at least for these compounds (including also ethyl benzene and xylenes, i.e., the BTEX group) the traffic component is highly significant [31,32]. In a recent paper [33] it has been argued that naphthalene, above ranked as 23 appears as a suitable as a VOC marker. However, the present study does not aim at elucidating reaction pathways to the various VOCs included.

It is further worthwhile to mention that the average height uncertainties for the single VOCs (Table 3) are relatively low. Thus, the ranking, although based on an averaging process is relatively close to a strong linear order, again as a result of the abovementioned indicator intercorrelation.

Typically it might be expected that the overall variation of the VOCs at the six indicator sites would follow a pattern that could be denoted as the mainstream [19]. However, in certain cases this appears not to be the case. Such peculiarities can be elucidated through application of a special module of the PyHasse software [21]. In the present case we looked for VOCs that did fall outside the mainstream on a 95% level [17,21] or in other words 95% of the VOCs were found to be within the defined mainstream [16,20].

At the 95% level only 2 'peculiar' VOCs were disclosed, i.e., No. 5 (isopentane) and No. 21 (propylene). The profiles for the two compounds were found to be [1, 1, 0, 1, 0, 1] and [0, 1, 0, 1, 0, 0], respectively. Hence, it can be concluded that isopentane was found to be surprisingly lower than the mainstream for site 3 and 6 whereas propylene apparently was surprisingly higher than expected at sites 2 and 4, respectively. Isopentane as well as propylene may come from both natural and artificial sources such as natural product from vegetation, natural gas, combustion of organic matter as well in tobacco smoke and in the exhaust of motor vehicles. A priori these peculiarities should be explained based on the actual characteristics of the mentioned sites. However, the available information does not allow that for the present.

3.2. Introducing the toxicity measure

The above analyses are based on the concentrations only. However, in order to assess the actual hazard towards humans it is necessary to adjust the concentration measures by appropriate toxicity data. In the present study the probability of the compounds to exhibit respiratory toxicity has been chosen as an illustrative example (cf. Table 1). Obviously other toxicity data could just as well be used depending on the actual effect towards the population that is studied. Hence, the MIS for this part of the study is obtained by multiplying the concentration data for the single compounds with the corresponding toxicity measure. Applying this MIS the Hasse diagram shown in Figure 3 is generated.

It is noted that the Hasse diagram (Figure 3) now appears less slim and less high with only 11 levels. However, a visual inspection easily discloses that the two diagrams (Figure 1 and 3) appear rather similar. This is clearly a result of the values applied for the respiratory toxicity (Table 1) that are found relatively close.

Some minor variations in the relative importance of the six sites can be noted. Thus, it is found that the relative importance of the six sites is Site 1 > Site 4 > Site 3 > Site 6 > Site 2 > Site 5, the corresponding normalized values being 0.310, 0.276, 0.161, 0,138, 0,092, 0.023, respectively. Apparently only the sites 3 and 4 have been interchanged.

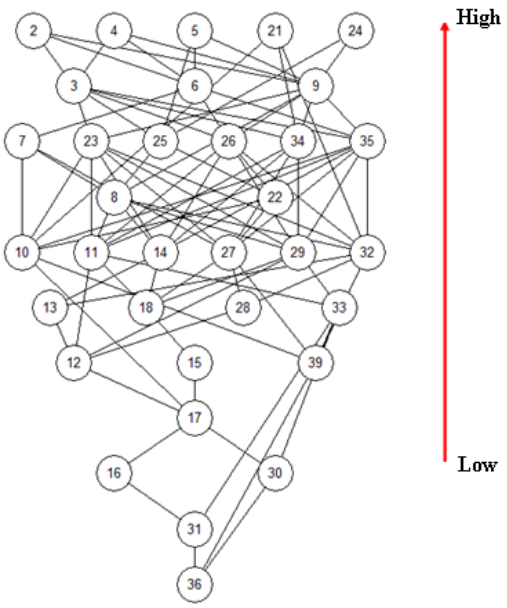

Figure 3. Hasse diagram based on the toxicity adjusted MIS (cf. Table 1). The diagram has 436 comparabilities and 125 incomparabilities.

Due to the above argument, it was expected that only minor variations in the average heights and ranks would be observed by introducing the toxicity measure. This assumption was verified by calculation the average heights and ranks based on the toxicity adjusted MIS (Table 4). It is noted that the average height uncertainty in this case is somewhat more pronounced. Obviously applying another toxicity adjustment with larger variations than the here sued may change the picture significantly. However, this is outside the scope of the present study. The comparison between the two rankings is visualized in Figure 4.

Table 4. Average heights and corresponding ranking of the 34 VOCs based on the original MIS adjusted for the probability for respiratory toxicity (cf. Table 1).

VOC	ID	Average height	Average height uncertainty	Rank
Propane	2	32.883	30...34	1.5
n-Butane	4	32.883	30...34	1.5
Isopentane	5	32.459	29...34	3
Toluene	24	31.778	27...34	4
Isobutane	3	29.542	26...32	5
Propylene	21	28.689	20...34	6
n-Pentane	6	28.646	24...31	7
n-Hexane	9	27.979	25...30	8
Ethyl benzene	25	25.317	21...29	9
2-Methyl pentane	7	24.758	20...30	10
m.p-Xylene	26	23.417	20...27	11
Benzene	23	23.233	19...28	12
Methylethylketone	35	22.619	19...27	13

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Ethylacetate	34	21.639	17...27	14
3-Methyl pentane	8	20.694	17...25	15
1.Isobutene	22	19.659	13...25	16
1.2.4-Trimethyl benzene	32	16.302	10...20	17
n-Heptane	11	15.931	11...19	18.5
p-Ethyl toluene	29	15.931	11...19	18.5
n-Decane	14	15.856	10...19	20
o-Xylene	27	15.431	11...19	21
Methylcyclopentane	10	13.021	7...20	22
n-Nonane	13	10.74	7...17	23
m-Ethyl toluene	28	10.493	7...16	24
Naphthalene	33	10.283	5...17	25
n-Tetradecane	18	9.98	7...14	26
n-Undecane	15	7.865	6...13	27
n-Octane	12	7.346	6...11	28
n-Tridecane	17	5.517	5...7	29
p-Dichlorobenzene	39	4.719	2...12	30
n-Dodecane	16	3.944	3...6	31
o-Ethyl toluene	30	2.944	2...5	32
1.3.5-Trimethyl benzene	31	2.433	2...4	33
n-Nonylaldehyde	36	1	1...1	34

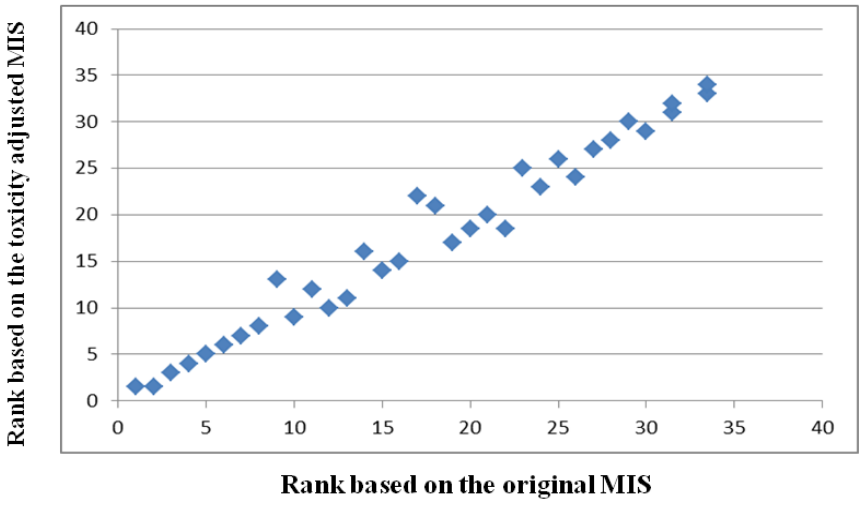

Figure 4. Correlation between the ranks based on the original MIS and the toxicity adjusted MIS.

3.3. The possible effect of data uncertainty

Looking at the data originally reported ([5], Table 2) it is obvious that the data are associated with a significant uncertainty. In a recent paper [23], we introduced a fuzzy-like approach to study the possible influence of data noise/uncertainty on the overall ranking of the elements in a MIS. Hence, in the present

study the influence of data uncertainties 0, 10, 25, 50, 75 and 100%, respectively, were investigated assuming a uniform distribution of the data around the original data (Table 1).

As usual in fuzzy concepts a parameter is needed to perform the defuzzification within the final step. According to Van de Walle et al. [34] this parameter is called α-cut. For very low α-cuts, virtually all variations are accepted, ultimately an α-cut = 0 means that all compounds will be regarded as equivalent, whereas for high α-cuts only "stable" comparisons remain. For each uncertainty level, we looked at the resulting Hasse diagram and the average height of the 34 compounds for α- cut = 0.1 and 0.9 to visualize the effect of α-cuts [23].

A rather surprising result of the uncertainty analyses is that independently of uncertainty level (apart from 100% level with α-cut = 0.9) and of α-cut, the average heights of the single compounds exhibit only very minor variations (Figure 5).

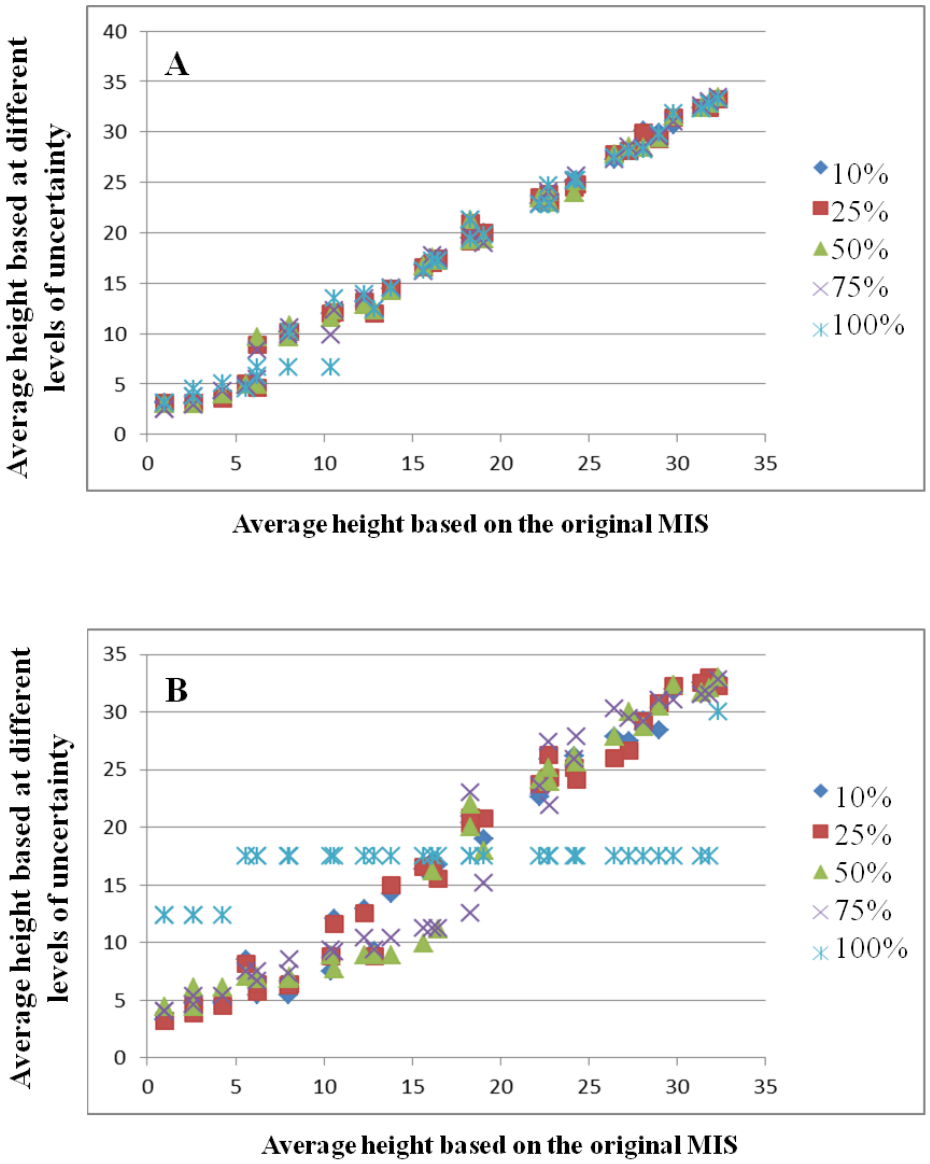

Figure 5. Average heights at different uncertainty levels as function of average height of the original MIS. A: α-cut = 0.1, B: α-cut = 0.9.

The apparent striking inertia of the compounds with respect to data uncertainty is the result of many steps not least the averaging process following a large (here 10,000) Monto Carlo runs. This is further discussed elsewhere [35].

In the present context it may be concluded that for a ranking purpose the actual uncertainty play a minor role. However, it should be noted that the here applied procedure is based on an indicator based uncertainty. Possibly a more diverse picture could develop following a procedure where the actual uncertainty for the single compounds (cf. [5], Table 2) was taken into account. Such calculations are for the time being not possible. However, the here presented data call for further development of the software package.

4. Conclusions

It has been illustrated how partial order methodology advantageously be used to assess the potential risk of chemical pollution here exemplary illustrated by VOC pollution in Yokohama, Japan. A major advantage of applying partial order methodology is that data may be applied without any pre-treatment. Further the mathematical basis is rather simple being based on the "≤" relation only.

Through the partial ordering it has been possible to rank the 34 compounds included in the study based on their atmospheric concentrations at 6 different sites, as indicators in Yokohama. Further it has been shown how toxicological measures as, e.g., the probability of the compounds to exhibit respiratory toxicity can be introduced and hereby creating a ranking based on toxicity adjusted concentrations. It should be noted that in the present exemplary case the respiratory toxicity has been studied. However, other effects may obviously be analyzed analogously.

Specific modules of the PyHasse software was applied to disclose the relative importance of the sites in the overall ranking of the VOCs as well as disclosing so-called 'peculiar' VOCs, i.e., VOCs that appear extremely high or low at certain sites.

Air pollution data are typically associated with a significant uncertainty. In a final section of the paper the possible effect on the ranking as a consequence of data uncertainty or data noise has been discussed. It was shown that overall the ranking was virtually unaffected by the data uncertainty. This phenomenon that may seem somewhat surprising will be further dealt with in future studies.

Conflicts of interest

Author declares no conflict of interest in this paper.

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