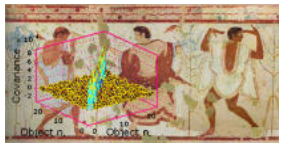

Chemometry Helps Visualizing Air Pollution

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Abstract

Two main pollutants are of significant importance: ozone and particulate matter. Automatic working instruments can help to monitor the concentrations in air. But such monitoring stations are expensive and therefore limited in number. Passive samplers are simple, inexpensive and could be placed in a large number over a wide area, they are part of european regulations (CEN/T 264) already. In combination with geostatistic methods like kriging they can show the pattern of the pollution and allow to find the optimal places to situate the monitoring stations after these studies.

Mass spectrometry allow the analysis of collected dust samples and even the analysis of single particles. In a similar manner the distribution of chemical elements in particles could be also depicted by geostatistics e.g. in a city area. Multivariate statistics, like biplots, allow the interpretation which sources contribute mainly to the particles.

Materials & Methods

For shortness only the references were given, details are therein. For the passive sampler to measure ozone the reaction of indigo to isatin was used as described in reference [1], with a period of exposure of 14 days.

The analysis of single dust particles were described in reference [2]. For the bulk analsis the PM10 fraction was collected on an ultrapure quartz filter and digested with nitric acid in a microwave oven. For the elemental analysis an Agilent ICP-MS 7500c spectrometer was used [3].

For the statistics commercially available programs were applied. For the isopleths (kriging) the Surfer program (Golden Software Inc., CO, USA) was used, for the principal component analysis (biplots) the Simca package (Pattern Recognition Systems, Bergen, Norway) [4].

Results

Example 1 : Ozone in a City Area

For the study of an integral coverage of ozone the Klagenfurt city basin was chosen. About 80 samplers, covered with the paper impregnated with indigo were distributed in this area measuring about 8 x 8 km. The median of six periodes were calculated and used as the geostatistic input. Fig. 1 shows the surfaces of equal pollution.

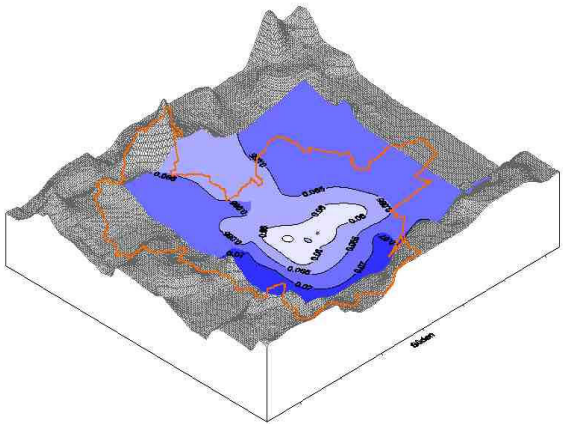

Fig.1 Distribution of ozone in the city basin of Klagenfurt. The red line is the city border.

Kriging in geostatistics needs reasonable modelling otherwise the use of a program like a black box leads to artefacts. In our example one can see that at the inner regions of the city where most of the pollution of the precurser (nitrogen oxides) were found, the concentration is lower (lighter colours) whereas towards the outer regions more ozone is formed. This agrees with the common knowledge written in every environmental textbook.

Example 2 : Chemical Elements in Single Particles.

Laser microprobe mass analysis allows the analysis of very small particles with a diameter of around

5 μm. As no quantification in units of mass was possible we have chosen as a measure how often an element occurred in particles. At about 50 sampling points we collected these particles with a selfmade impactor. Geostatistics which shows lines of equal occurrence of an marker element indicates in the center of the lines the source of the pollutant.

Example 3 : Bulk Analysis of Dust.

Nowadays analytical tools like mass spectrometer provide hugh amounts of information, for elemental analysis almost the whole periodic table. Supposed we collect dust at 20 sampling points and analyse the concentration of 40 elements 800 numbers turn up in our data sheet. It goes beyond human skills to recognize any structures in this vast array without applying chemometric methods. To reduce the dimension principal component analysis PCA is an approved choice. As an unsupervised classification resp. cluster analysis it avoids that results are produced intendedly, an important aspect in environmental chemistry which often has to be presented at court.
Fig. 2 shows the biplot for different sampling situations, including roadside, clean air areas, kindergarden, flats and a pub full of tabacco smoke. Further procedure, e.g. removal of the more outlying points would give more detail for the other sampling points. It is interesting that at a first glance the PCA gives the right marker elements for a certain type of pollution: for the traffic Pt from the catalyst, Zn from the tyres, which replaced the lead we had in the past; K, Cd and Tl for tabacco smoke. This assignments may be a starting point to do more sophisticated statistical analysis like chemical mass balance. It gives the first hints which data set should be involved.

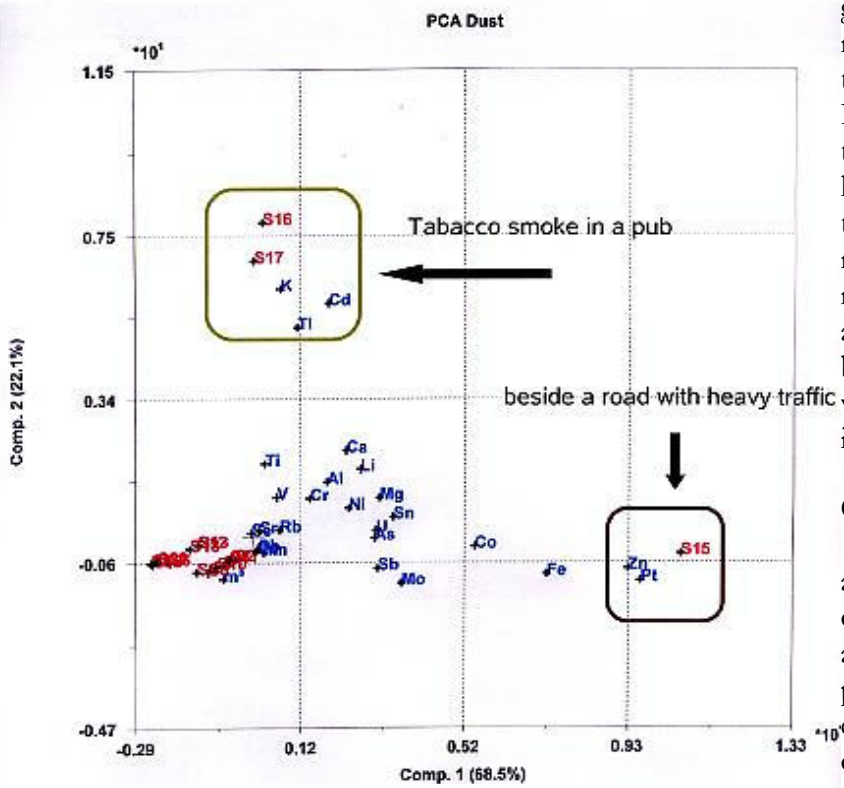

Fig. 2 PCA analysis of 20 samples with 27 elements

Conclusions

Chemometric methods are a very important tools to combine landscape with analytical data gained at sampling points. The visualization allows even non experts to realize a certain situation and may help politicians to change it. Chemometry has become an intrinsic part of analytical chemistry and therefore should be included in the curriculum. For master studies this education should go beyond simple statistics.

References

1) P. Remler, W. Kosmus, Integrale Langzeitmethode zur Bestimmung von Ozon in der Atmosphäre, Fresen J. Anal. Chem., 329(8) (1988) 871-876
2) R. Wippel, G. Haas, W. Kosmus, The analysis of dust particles in Graz, Austria, Forum Städte-Hygiene, 47, (1996) 219-224
3) N. Fellner, S. Findenig, Ch. Kurta, T. Schmalzbauer, M. Schmidt, Tutorial in environmental studies, KF-University Graz (2007), unpublished results.
4) S. Wold, Pattern recognition by means of disjoint principal component models, Pattern Recognition, 8(3) (1976) 127-139