Analytical Challenges in Environmental and Geosciences

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New emerging issues in environmental science can often be linked to the development of new analytical techniques and methods. A prominent example is the introduction of the electron capture detector in the 1960s. The electron capture detector is a highly selective and sensitive detector for halogenated compounds and opened an analytical window for the investigation of the ubiquitous occurrence of halogenated insecticides such as DDT and polychlorinated biphenyls in environmental matrices and animal tissues.

In the last 15 years the rapid development of liquid chromatography–mass spectrometry (LC-MS) instruments with increasing sensitivity and selectivity has opened another analytical window for polar, not well degradable water pollutants. Among these so-called new emerging pollutants are pharmaceuticals and personal care products (PhPCPs), a very large and diverse group of chemicals occurring in the water cycle. A recent publication of the German Federal Environment Agency (Umweltbundesamt) reports on monitoring data for more than 270 pharmaceuticals and their metabolites in the literature. The challenge in the analysis of PhPCPs and other new emerging compounds is the selection of the most relevant compounds from a huge list of chemicals in daily use. In Europe this list comprises several tens of thousands of compounds from a total of more than 120,000 registered chemicals. The consideration of metabolites and abiotic transformation products of the original pollutants in surface water and groundwater and in wastewater and

drinking water treatment further increases the number of relevant compounds and requires detailed knowledge of chemical and biological transformation processes. In environmental science the general questions for analytical chemists are still the same as 25 years ago during my university education: what compounds occurs in what quantity, where, and why? Preferably, sensitive and selective analytical methods are the basis to answer these questions. Most important today, especially for organic pollutants, are separation techniques such as gas chromatography–mass spectrometry and LC-MS. Other approaches include classic and miniaturized applications of spectroscopy, electrochemistry, or molecular recognition by antibodies or specific natural or synthetic receptors. The latter are also important in effect-directed analysis, which aims to link biological effects to compound identification and quantitation. Immunoassays such as enzyme-linked immunosorbent assays are very useful tools for rapid, inexpensive, and portable detection of specific analytes. The challenge is still the generation of specific antibodies for a broader range of relevant compounds.

Multicompound detection and identification is the domain of nontarget approaches by high-resolution mass spectrometry, which is based on the determination of the molecular formulae and has experienced increasing application owing to recent developments of sensitive and reliable quadrupole time-of-flight and Orbitrap instruments. The main challenges are the selection of relevant signals from the large data sets and the elucidation of the compound structures of unknowns. This requires statistical approaches to select compounds of interest and further structural information from mass fragmentation and often nuclear magnetic resonance (NMR) spectroscopy to elucidate structural isomers. Despite increased NMR sensitivity, there is still a

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large gap in sensitivity between NMR and LC-MS. Another very promising mass-spectrometric approach in environmental science is compound-specific stable isotope analysis, which is used to determine the sources and transformation processes of organic pollutants. For example, the isotopic fractionation of carbon, hydrogen, and nitrogen can be used to distinguish between abiotic hydrolysis and biotransformation of the herbicide isoproturon. However, before compound-specific stable isotope analysis can be applied for polar compounds in environmental samples, the limitations of sensitivity and the coupling with separation by liquid chromatography have to be overcome. A further approach to link contamination to different sources or to reveal environmental transport is the use of pollutants as rather specific indicators. Much work has been done to show the impact of wastewater effluents on surface water and groundwater using pharmaceuticals, caffeine, or artificial sweeteners as wastewater indicators. A further challenge is to find and select a set of suitable and widely occurring compounds for the distinction and quantification of different environmental processes.

This special issue on Analytical Challenges in Environmental and Geosciences includes a rather selective compilation of review articles, original articles, and technical notes.

The compilation of subjects is far from complete, but reflects major issues of and gives specific insights into analytical applications in environmental science. The articles present methods, views, developments, and applications of analytical chemistry to elucidate the occurrence and fate of trace pollutants in the environment.

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